Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1600RXA

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

| | | |
|---|---|---|
| NEWS 1 | | Web Page URLs for STN Seminar Schedule - N. America |
| NEWS 2 | | "Ask CAS" for self-help around the clock |
| NEWS 3 | SEP 09 | CA/CAplus records now contain indexing from 1907 to the present |
| NEWS 4 | DEC 08 | INPADOC: Legal Status data reloaded |
| NEWS 5 | SEP 29 | DISSABS now available on STN |
| NEWS 6 | OCT 10 | PCTFULL: Two new display fields added |
| NEWS 7 | OCT 21 | BIOSIS file reloaded and enhanced |
| NEWS 8 | OCT 28 | BIOSIS file segment of TOXCENTER reloaded and enhanced |
| NEWS 9 | NOV 24 | MSDS-CCOHS file reloaded |
| NEWS 10 | DEC 08 | CABA reloaded with left truncation |
| NEWS 11 | DEC 08 | IMS file names changed |
| NEWS 12 | DEC 09 | Experimental property data collected by CAS now available in REGISTRY |
| NEWS 13 | DEC 09 | STN Entry Date available for display in REGISTRY and CA/CAplus |
| NEWS 14 | DEC 17 | DGENE: Two new display fields added |
| NEWS 15 | DEC 18 | BIOTECHNO no longer updated |
| NEWS 16 | DEC 19 | CROPU no longer updated; subscriber discount no longer available |
| NEWS 17 | DEC 22 | Additional INPI reactions and pre-1907 documents added to CAS databases |
| NEWS 18 | DEC 22 | IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields |
| NEWS 19 | DEC 22 | ABI-INFORM now available on STN |
| NEWS 20 | JAN 27 | Source of Registration (SR) information in REGISTRY updated and searchable |
| NEWS 21 | JAN 27 | A new search aid, the Company Name Thesaurus, available in CA/CAplus |
| NEWS 22 | FEB 05 | German (DE) application and patent publication number format changes |
| NEWS 23 | MAR 03 | MEDLINE and LMEDLINE reloaded |
| NEWS 24 | MAR 03 | MEDLINE file segment of TOXCENTER reloaded |
| NEWS 25 | MAR 03 | FRANCEPAT now available on STN |

| | |
|---|---|
| NEWS EXPRESS | MARCH 5 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004 |
| NEWS HOURS | STN Operating Hours Plus Help Desk Availability |
| NEWS INTER | General Internet Information |
| NEWS LOGIN | Welcome Banner and News Items |
| NEWS PHONE | Direct Dial and Telecommunication Network Access to STN |
| NEWS WWW | CAS World Wide Web Site (general information) |

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:02:25 ON 29 MAR 2004

=> fil reg
COST IN U.S. DOLLARS

| | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 09:02:32 ON 29 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 MAR 2004 HIGHEST RN 668418-93-7
DICTIONARY FILE UPDATES: 28 MAR 2004 HIGHEST RN 668418-93-7

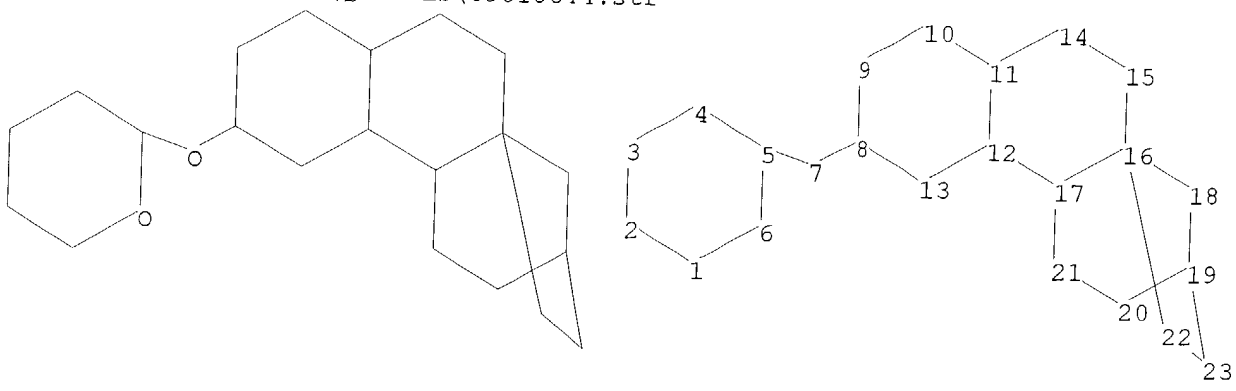
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\STNEXP4\QUERIES\09810644.str



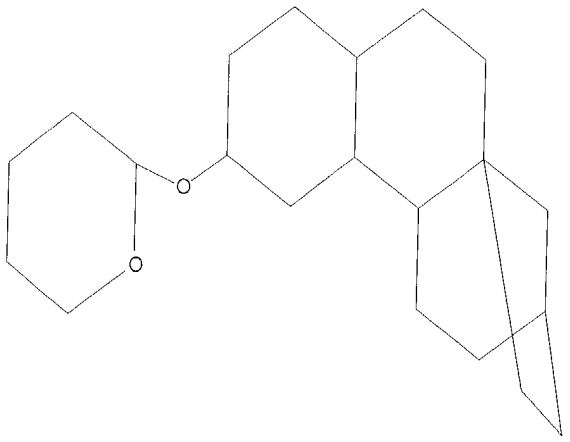

chain nodes :
7
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
chain bonds :

5-7 7-8
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 11-14 12-13 12-17
14-15 15-16 16-17 16-18 16-22 17-21 18-19 19-20 19-23 20-21 22-23
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 7-8 8-9 8-13 9-10 10-11 11-12 11-14 12-13
12-17 14-15 15-16 16-17 16-18 16-22 17-21 18-19 19-20 19-23 20-21 22-23

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR




Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 09:02:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 138 TO ITERATE

100.0% PROCESSED 138 ITERATIONS 12 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2056 TO 3464
PROJECTED ANSWERS: 33 TO 447

L2 12 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 09:02:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2793 TO ITERATE

100.0% PROCESSED 2793 ITERATIONS 179 ANSWERS
SEARCH TIME: 00.00.01

L3 179 SEA SSS FUL L1

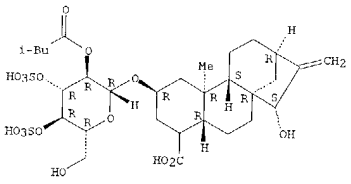
=> s l3 and caplus/lc
34527749 CAPLUS/LC
L4 168 L3 AND CAPLUS/LC

=> s l3 not l4
L5 11 L3 NOT L4

=> d l5 1-11

L5 ANSWER 1 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
RN 102130-43-8 REGISTRY
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,15α)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-2,10a-Ethanophenanthrene, 19-norkaur-16-en-18-oic acid deriv.
FS STEREOSEARCH
MF C30 H46 O16 S2 . 2 K
SR CAS Client Services
LC STN Files: BEILSTEIN*, CHEMCATS, CSCHEM
(*File contains numerically searchable property data)

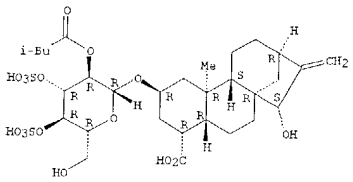
Absolute stereochemistry.



●2 K

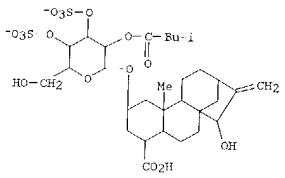
L5 ANSWER 2 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
RN 100938-11-2 REGISTRY
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, disodium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-2,10a-Ethanophenanthrene, 19-norkaur-16-en-18-oic acid deriv.
FS STEREOSEARCH
MF C30 H46 O16 S2 . 2 Na
SR CAS Client Services
LC STN Files: CHEMCATS, CSCHEM
CRN (1398-13-6)

Absolute stereochemistry.

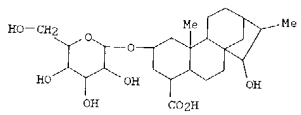


●2 Na

L5 ANSWER 3 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
RN 22956-67-8 REGISTRY
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-α-D-glucopyranosyl]oxy]-, ion(2-), (2β,4α,15α)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 19-Norkaur-16-en-18-oic acid, 2β-(α-D-glucopyranosyloxy)-15α-hydroxy-, 3',4'-bis(hydrogen sulfate) 2'-isovalerate, ion(2-) (8CI)
CN 1H-2,10a-Ethanophenanthrene, 19-norkaur-16-en-18-oic acid deriv.
MF C30 H44 O16 S2

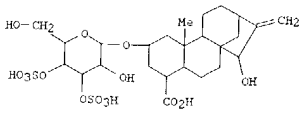


L5 ANSWER 4 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
RN 22007-76-7 REGISTRY
CN 19-Norkauran-18-oic acid, 2-(α-D-glucopyranosyloxy)-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-2,10a-Ethanophenanthrene, 19-norkauran-18-oic acid deriv.
MF C25 H40 O9



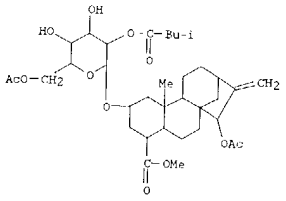
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L5 ANSWER 5 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
RN 18558-58-2 REGISTRY
CN Apoatractyloside, dibarium salt (8CI) (CA INDEX NAME)
MF C25 H38 O15 S2 . 2 Ba
LC STN Files: BEILSTEIN*
(*File contains numerically searchable property data)
CRN (25127-19-9)



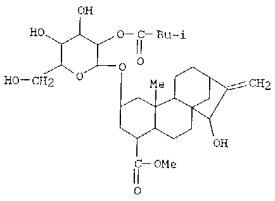
●2 Ba

L5 ANSWER 6 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
RN 18467-03-3 REGISTRY
CN Atractylin, methyl ester, 6',15-diacetate 2'-isovalerate (8CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Isovaleric acid, 2'-ester with atractylin methyl ester 6',15-diacetate
OTHER NAMES:
CN Di-O-acetylisovalerylatractyline methyl ester
MF C35 H52 O12



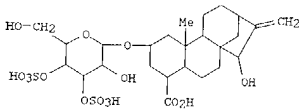
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L5 ANSWER 7 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
RN 18467-01-1 REGISTRY
CN Atractylin, methyl ester, 2'-isovalerate (8CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Isovaleric acid, 2'-ester with atractylin methyl ester
OTHER NAMES:
CN Isovalerylatractyline methyl ester
MF C31 H48 O10
LC STN Files: BEILSTEIN*
(*File contains numerically searchable property data)



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

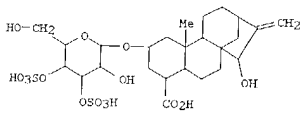
L5 ANSWER 8 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
RN 17631-43-5 REGISTRY
CN 19-Norkaur-16-en-18-oic acid, 2-[(3,4-di-O-sulfo-α-D-glucopyranosyl)oxy]-15-hydroxy-, calcium potassium salt, (2β,4β,15α)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-2,10a-Ethanophenanthrene, 19-norkaur-16-en-18-oic acid deriv.
CN Apoatractyloside, calcium potassium salt (1:1:1) (8CI)
MF C25 H38 O15 S2 . Ca . K
CRN (17605-50-4)



● Ca

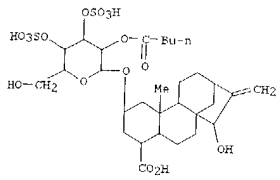
● K

L5 ANSWER 9 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
RN 17605-50-4 REGISTRY
CN 19-Norkaur-16-en-18-oic acid, 2-[(3,4-di-O-sulfo-α-D-glucopyranosyl)oxy]-15-hydroxy-, (2β,4β,15α)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 18-Norkaur-16-en-19-oic acid, 2β-(α-D-glucopyranosyloxy)-15α-hydroxy-, 3',4'-bis(hydrogen sulfate) (8CI)
CN 1H-2,10a-Ethanophenanthrene, 19-norkaur-16-en-18-oic acid deriv.
MF C25 H38 O15 S2
CI COM
LC STN Files: BEILSTEIN*
(*File contains numerically searchable property data)



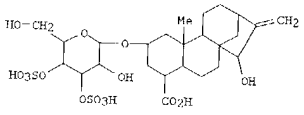
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L5 ANSWER 10 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
RN 17605-43-5 REGISTRY
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(1-oxopentyl)-3,4-di-O-sulfo-α-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-2,10a-Ethanophenanthrene, 19-norkaur-16-en-18-oic acid deriv.
MF C30 H46 O16 S2



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L5 ANSWER 11 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
RN 17605-35-5 REGISTRY
CN 19-Norkaur-16-en-18-oic acid, 2-[(3,4-di-O-sulfo-α-D-glucopyranosyl)oxy]-15-hydroxy- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-2,10a-Ethanophenanthrene, 19-norkaur-16-en-18-oic acid deriv.
MF C25 H38 O15 S2
LC STN Files: BEILSTEIN*
(*File contains numerically searchable property data)



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

=> fil caplus
COST IN U.S. DOLLARS

| | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 180.16 | 180.37 |

FILE 'CAPLUS' ENTERED AT 09:04:31 ON 29 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


FILE COVERS 1907 - 29 Mar 2004 VOL 140 ISS 14
FILE LAST UPDATED: 28 Mar 2004 (20040328/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l4
L6 449 L4

=> s l4 and (Anderson C? or Davis R? or CLevenger W? or Wiley S? or Miller S? or Szaba T? or Ghosh S? or Moos W? or Pei Y?)/au
449 L4
2676 ANDERSON C?/AU
5599 DAVIS R?/AU
46 CLEVENGER W?/AU
68 WILEY S?/AU
3716 MILLER S?/AU
0 SZABA T?/AU
4551 GHOSH S?/AU
140 MOOS W?/AU
621 PEI Y?/AU
L7 9 L4 AND (ANDERSON C? OR DAVIS R? OR CLEVENGER W? OR WILEY S? OR MILLER S? OR SZABA T? OR GHOSH S? OR MOOS W? OR PEI Y?)/AU

=> d ibib abs hitstr l7 1-9

L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:465960 CAPLUS
DOCUMENT NUMBER: 137:47439
TITLE: Preparation of amino acid derivatives for altering mitochondrial function and cellular responses
INVENTOR(S): **Pei, Yazhong; Moos, Walter H.; Ghosh, Soumitra S.**
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2002048092 | A2 | 20020620 | WO 2001-US48068 | 20011214 |
| WO 2002048092 | A3 | 20030109 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BR, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2002039595 | A5 | 20020624 | AU 2002-39595 | 20011214 |
| US 2002173543 | A1 | 20021121 | US 2001-20090 | 20011214 |
| US 6552076 | B2 | 20030422 | | |

PRIORITY APPLN. INFO.: US 2000-255803P P 20001215
WO 2001-US48068 W 20011214
OTHER SOURCE(S): MARPAT 137:47439

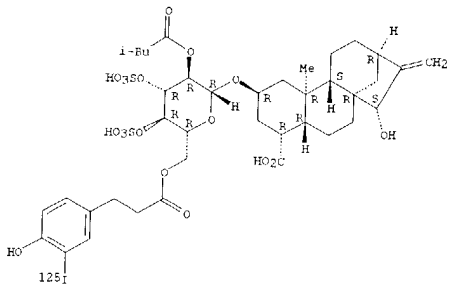
AB Compds. R1COCHR2N(CH2CO2H)CO-A-C6H4NHCOR3 [A is a direct bond, (un)substituted alkyldiyl, -O-(alkyldiyl)-, -(alkyldiyl)-O-, -N(R')-(alkyldiyl)- (R' = H or alkyl), -(alkyldiyl)-N(R')-, heterocyclediyl, or heterocyclealkyldiyl; R1 = OH, alkoxy, aryloxy, arylalkyloxy, amino, or mono- or dialkylamino; R2 = H, (un)substituted alkyl, aryl, arylalkyl, heterocyclyl, or heterocyclylalkyl; R3 = (un)substituted alkyl, aryl, arylalkyl, heterocyclyl, or heterocyclylalkyl] were prepared for treating diseases by altering mitochondrial function that affects cellular processes. Thus, (HO2CCH2)2NCOC6H4NHAc-o was prepared by substitution reaction of glycine tert-Bu ester acetate with bromoacetate resin, reaction with 2-nitrobenzoic acid, nitro group reduction, acetylation with Ac2O, and resin cleavage using TFA. Biol. activities of compds. of the invention were examined in neuronal viability, displacement of an adenine nucleotide translocase ligand from isolated mitochondria, and chondrocyte cytodeprotection assays.

IT **437992-74-0**
RL: BSU (Biological study, unclassified); BIOL (Biological study) (radioligand; measurement of binding efficacy of amino acid derivs. in relation to mitochondrial function and cellular responses)

RN 437992-74-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-[4-hydroxy-3-(iodo-125I)phenyl]-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-

L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:406465 CAPLUS
DOCUMENT NUMBER: 137:197709
TITLE: High-throughput assessment of mitochondrial membrane potential in situ using fluorescence resonance energy transfer
AUTHOR(S): Nykens, James A.; Fleck, Beth; **Ghosh, Soumitra**; Lewis, Michelle; Velicelebi, Gonul; Ward, Manus W.
CORPORATE SOURCE: MitoKor, San Diego, CA, 92121, USA
SOURCE: Mitochondrion (2002), 1(5), 461-473
CODEN: MITOCN; ISSN: 1567-7249
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

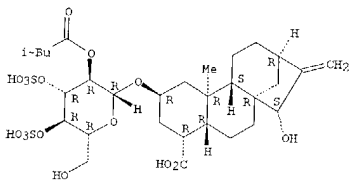
AB Mitochondrial dysfunction causes dozens of debilitating diseases, and is implicated in the etiol. of type 2 diabetes, Parkinson's, and Alzheimer's diseases, among others. However, development of mitochondrially targeted therapeutic agents has been impeded by the lack of high-throughput screening techniques that are capable of distinguishing in intact cells the mitochondrial membrane potential (ΔΨm) from the plasma membrane potential, (ΔΨp). We report here a fluorescence resonance energy transfer (FRET) assay that specifically monitors ΔΨm that is not confounded by background signal arising from potentiometric dye responding to ΔΨp. The technique relies on energy transfer between nonyl acridine orange (NAO), which stains diphosphatidyl glycerol (cardiolipin) that is indigenous to the inner mitochondrial membrane, and tetramethylrhodamine Me ester (TMR), a potentiometric dye that is sequestered by mitochondria as a Nernstian function of ΔΨm and concentration. FRET occurs only when both dyes co-localize to the mitochondria, and results in quenching of NAO emission by TMR in proportion to ΔΨm. Validation studies using compds. with well-characterized mitochondrial effects, including oligomycin, CCCP+, bongkrekic acid, cyclosporin A, nigericin, ADP, and ruthenium red, demonstrate that the FRET-based ΔΨm assay responds in accord with the known pharmacol. Validation studies assessing the suitability of the technique for high-throughput compound screening indicate that the assay provides a sensitive and robust assessment not only of mitochondrial integrity in situ, but also, when used in conjunction with agents such as cyclosporin A, an indicator of permeability transition.

IT **17754-44-8**, Atractyloside
RL: BSU (Biological study, unclassified); BIOL (Biological study) (high-throughput assessment of mitochondrial membrane potential in situ using fluorescence resonance energy transfer)

RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)




●2 K

REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:833514 CAPLUS
DOCUMENT NUMBER: 136:1609
TITLE: Production of adenine nucleotide translocator (ANT) with recombinant cells, ANT ligands and screening assays therefor
INVENTOR(S): **Anderson, Christen M.; Davis, Robert E.; Clevenger, William; Wiley, Sandra Eileen; Miller, Scott W.**; Szabo, Tomas R.; **Ghosh, Soumitra S.; Moos, Walter H.; Pei, Yazhong**; Carroll, Amy K.
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 147 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001085944 | A2 | 20011115 | WO 2001-US15416 | 20010511 |
| WO 2001085944 | A3 | 20020829 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1283884 | A2 | 20030219 | EP 2001-935420 | 20010511 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| JP 2003532420 | T2 | 20031105 | JP 2001-582533 | 20010511 |

PRIORITY APPLN. INFO.: US 2000-569327 A 20000511
WO 2001-US15416 W 20010511

OTHER SOURCE(S): MARPAT 136:1609

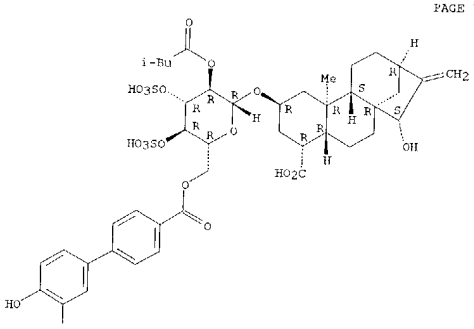
AB Compns. and methods are provided for producing adenine nucleotide translocator (ANT) polypeptides and fusion proteins, including the production and use of recombinant expression constructs having a regulated promoter. ANT ligands and compns. and methods for identifying ANT ligands, agents that bind ANT and agents that interact with ANT are also disclosed. Thus, ANT cDNAs were expressed in Sf9 and E.coli. Fluorescent and radiolabeled derivs. of atractyloside were prepared Binding of these derivs. to ANT was examined

IT **267886-33-9P 267886-35-1P 267886-37-3P**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(production of adenine nucleotide translocator (ANT) with recombinant cells, ANT ligands and screening assays therefor)

RN 267886-33-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxy-3-

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



PAGE 2-A

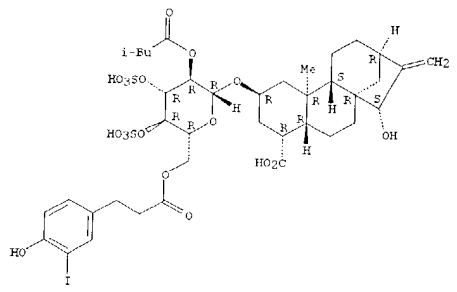


RN 267886-37-3 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-(4-hydroxy-3-iodobenzoyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
iodophenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

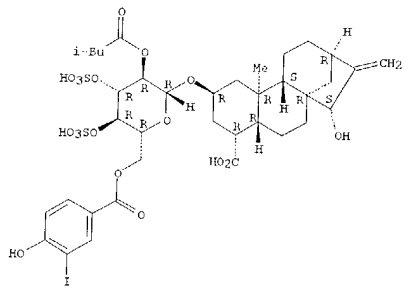
Absolute stereochemistry.



RN 267886-35-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[(4'-hydroxy-3'-iodo[1,1'-biphenyl]-4-yl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

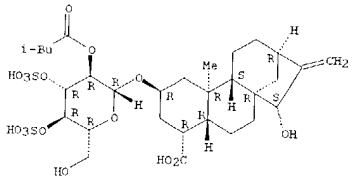
L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT **17754-44-8**, Atractyloside **267886-34-0**
**267886-55-5 374064-29-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(production of adenine nucleotide translocator (ANT) with recombinant cells, ANT ligands and screening assays therefor)

RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

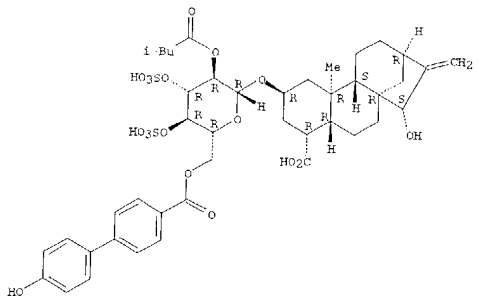


●2 K

RN 267886-34-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[(4'-hydroxy[1,1'-biphenyl]-4-yl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

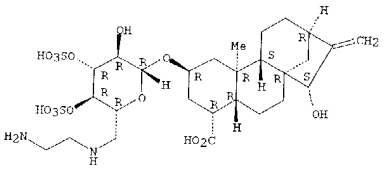
Absolute stereochemistry.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-55-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-[(2-aminoethyl)amino]-6-deoxy-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 374064-29-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, trihydrate, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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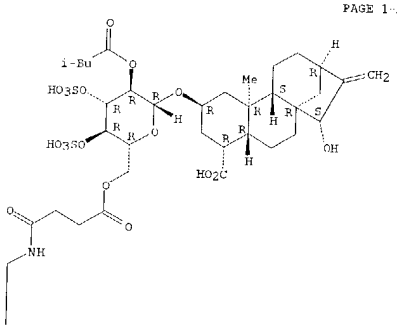
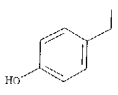


PAGE 2-A



RN 267886-48-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-deoxy-6-[[2-[[3-(4-hydroxyphenyl)-1-oxopropyl]amino]ethyl]amino]-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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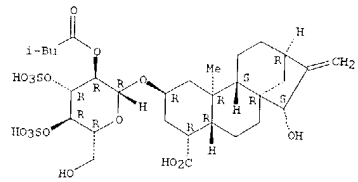


●2 K

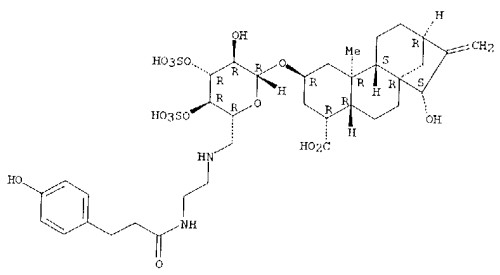
PAGE 2-A

●3 H2O

IT **267886-39-5P 267886-48-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(production of adenine nucleotide translocator (ANT) with recombinant cells, ANT ligands and screening assays therefor)
RN 267886-39-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-[[2-(4-hydroxyphenyl)ethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

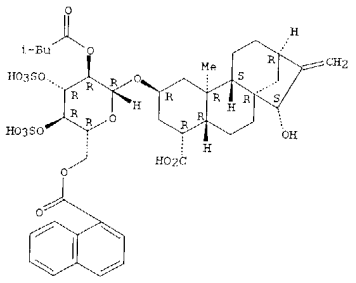
Absolute stereochemistry.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT **84882-67-7P 267886-16-8P 267886-17-9P**
**267886-18-0P 267886-19-1P 267886-21-5P**
**267886-32-8P 267886-36-2P 267886-38-4P**
**267886-40-8P 267886-41-9P 267886-42-0P**
**267886-43-1P 267886-44-2P 267886-45-3P**
**267886-46-4P 267886-47-5P 267886-49-7P**
**268557-13-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(production of adenine nucleotide translocator (ANT) with recombinant cells, ANT ligands and screening assays therefor)
RN 84882-67-7 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[(2-O-(3-methyl-1-oxobutyl)-6-O-(1-naphthalenylcarbonyl)-2,3-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

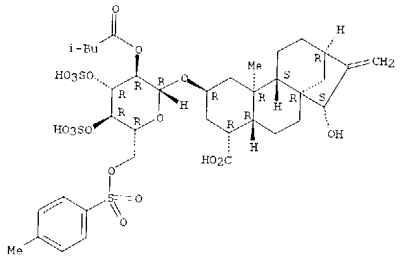
Absolute stereochemistry.



L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

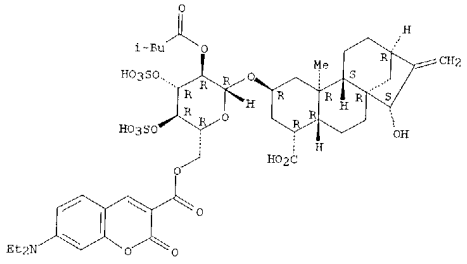
RN 267886-16-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-[(4-methylphenyl)sulfonyl]-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

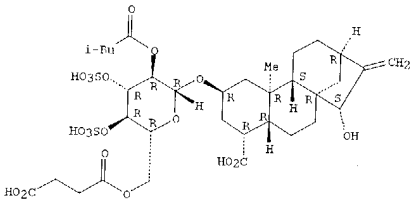


RN 267886-17-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[[7-(diethylamino)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



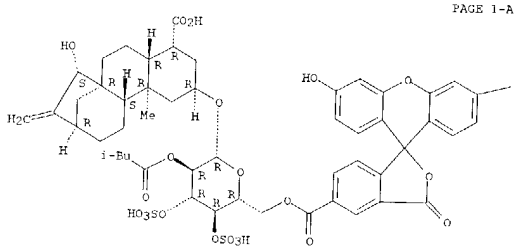
L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-32-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

-OH

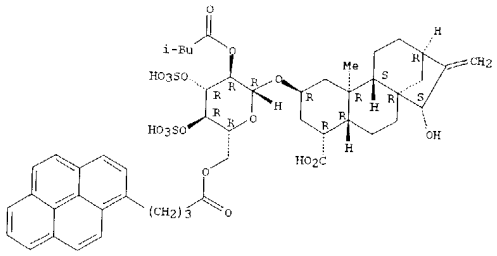
RN 267886-36-2 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-(4-hydroxybenzoyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

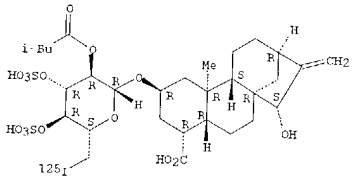
RN 267886-18-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-[1-oxo-4-(1-pyrenyl)butyl]-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 267886-19-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-deoxy-6-(iodo-125I)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

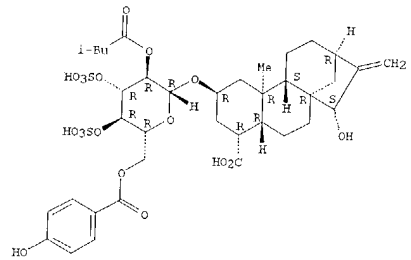
Absolute stereochemistry.



RN 267886-21-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-(3-carboxy-1-oxopropyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

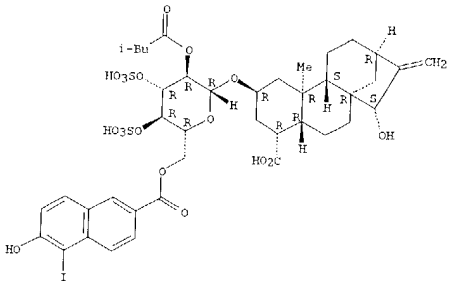
Absolute stereochemistry.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-38-4 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[(6-hydroxy-5-iodo-2-naphthalenyl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 267886-40-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-[[2-(4-hydroxy-3-iodophenyl)ethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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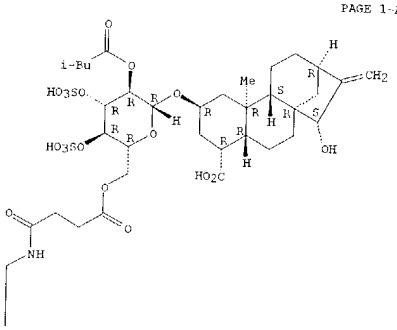
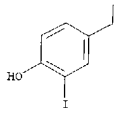


PAGE 2-A

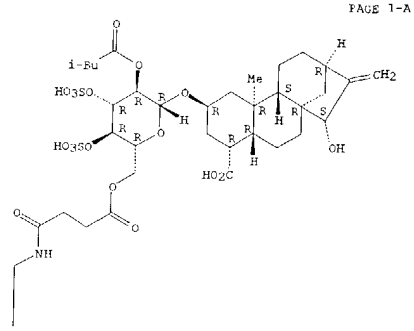


RN 267886-41-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-[[2-(4-hydroxy-3,5-diiodophenyl)ethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4aα,15α)- (9CI) (CA INDEX NAME)

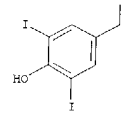
Absolute stereochemistry.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



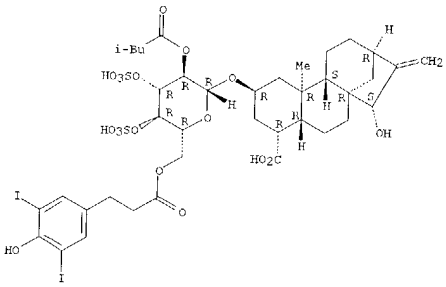
PAGE 2-A



RN 267886-42-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxy-3,5-diiodophenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4aα,15α)- (9CI) (CA INDEX NAME)

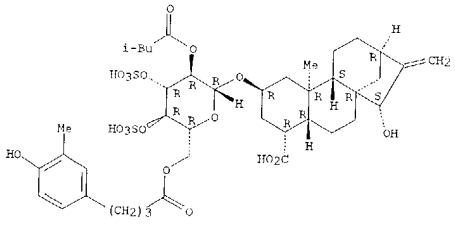
Absolute stereochemistry.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-43-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-(4-hydroxy-3-methylphenyl)-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4aα,15α)- (9CI) (CA INDEX NAME)

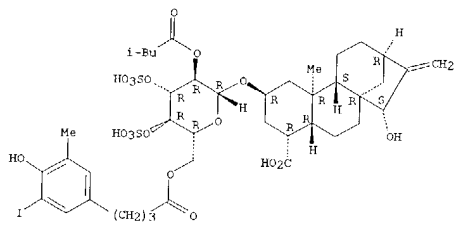
Absolute stereochemistry.



RN 267886-44-2 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-(4-hydroxy-3-iodo-5-methylphenyl)-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4aα,15α)- (9CI) (CA INDEX NAME)

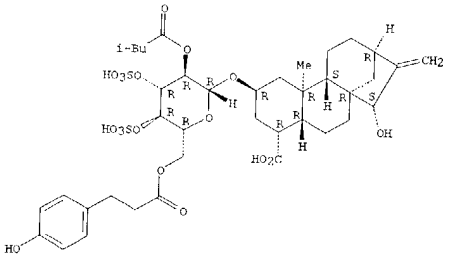
Absolute stereochemistry.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-45-3 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxyphenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4aα,15α)- (9CI) (CA INDEX NAME)

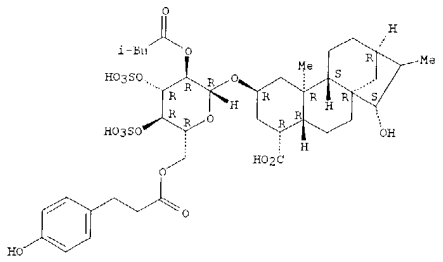
Absolute stereochemistry.



RN 267886-46-4 CAPLUS
CN 19-Norkauran-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxyphenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4aα,15α,16ξ)- (9CI) (CA INDEX NAME)

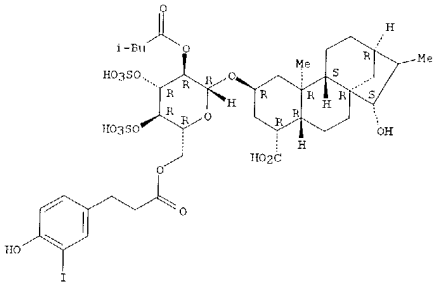
Absolute stereochemistry.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-47-5 CAPLUS
CN 19-Norkauran-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxy-3-iodophenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α,16ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 267886-49-7 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-deoxy-6-[[2-[[3-(4-hydroxy-3,5-diiodophenyl)-1-oxopropyl]amino]ethyl]amino]-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:338715 CAPLUS
DOCUMENT NUMBER: 134:349692
TITLE: Determining interactions of cyclophilin D and the adenine nucleotide translocator to assess mitochondrial permeability and in screening permeability altering substances
INVENTOR(S): Murphy, Anne N.; **Clevenger, William; Wiley, Sandra E.**; Andreyev, Alexander Y.; Frigeri, Luciano G.; Velicelebi, Gonul; **Davis, Robert E.**
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 186 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001032876 | A2 | 20010510 | WO 2000-US30535 | 20001103 |
| WO 2001032876 | A3 | 20020117 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 6562563 | B1 | 20030513 | US 1999-434354 | 19991103 |
| EP 1228206 | A2 | 20020807 | EP 2000-975595 | 20001103 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| JP 2003516128 | T2 | 20030513 | JP 2001-538558 | 20001103 |

PRIORITY APPLN. INFO.: US 1999-434354 A 19991103
WO 2000-US30535 W 20001103

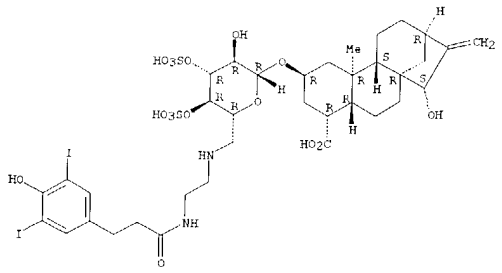
AB A method of measuring transitions in mitochondrial membrane permeability by assessing the interaction of the mitochondrial adenine nucleotide translocator and cyclophilin D is described. The method can be used to screen for permeability altering agents for use, for example, in the treatment of a variety of conditions associated with altered mitochondrial function. Hexahistidine-labeled ANT3 adenine nucleotide translocator manufactured by expression of the cloned gene in Trichoplusia ni cells was immobilized on nickel-containing agarose beads. Cyclophilin D was manufactured as a fusion protein with glutathione-S-transferase. The cyclophilin D fusion product was incubated with the bead immobilized ANT3 and the bound cyclophilin D was determined by immunoassay of the glutathione-S-transferase moiety. The interaction showed the expected properties.

IT **17754-44-8**, Atractyloside
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(as modulator of mitochondrial membrane permeability; determining interactions of cyclophilin D and adenine nucleotide translocator to assess mitochondrial permeability and in screening permeability altering substances)

RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-

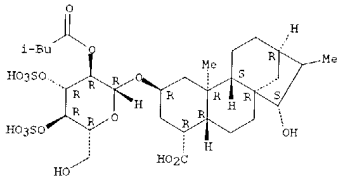
L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Absolute stereochemistry.



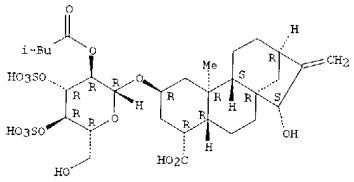
RN 268557-13-7 CAPLUS
CN 19-Norkauran-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α,16ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 K

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:168189 CAPLUS
DOCUMENT NUMBER: 134:219377
TITLE: Methods for assaying mitochondrial intermembrane space protein translocation and drug screening
INVENTOR(S): Murphy, Anne N.; **Wiley, Sandra Eileen;** Andreyev, Alexander Y.
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 70 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001016373 | A2 | 20010308 | WO 2000-US23638 | 20000828 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 1999-151231P P 19990827
US 1999-169508P P 19991207
US 2000-606370 A 20000628

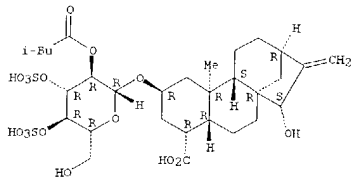
AB Compns. and methods are provided for identifying agents that alter mitochondrial intermembrane space protein (MISP) translocation. The screening methods generally detect agents that alter the level of detectable extramitochondrial MISP following exposure of a cell to an agent known or suspected to induce mitochondrial intermembrane space protein translocation. Such agents may be used, for example, in the treatment of a variety of conditions associated with altered mitochondrial function. SH-SY5Y neuroblastoma cells were transfected with a recombinant expression construct encoding adenylate kinase-2 fusion protein with hemagglutinin epitope tag. Several stable cell lines were established that overexpress the fusion protein. The cells were treated with various apoptogens, harvested, and analyzed by Western blot for cytochrome c and adenylate kinase release from the mitochondria.

IT **17754-44-8**, Atractyloside **33286-30-5**, Carboxyatractyloside
RL: BAC (Biological activity or effector, except adverse); EPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(methods for assaying mitochondrial intermembrane space protein translocation and drug screening)

RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

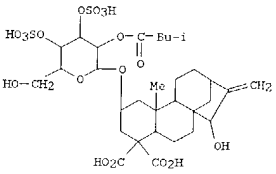
Absolute stereochemistry.

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 K

RN 33286-30-5 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,15α)- (9CI) (CA INDEX NAME)



●2 K

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:911534 CAPLUS
DOCUMENT NUMBER: 134:66121
TITLE: Compositions and methods for assaying subcellular conditions and processes using energy transfer for drug screening
INVENTOR(S): Dykens, James A.; Velicelebi, Gonul; **Ghosh, Soumitra S.**
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 189 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000079274 | A2 | 20001228 | WO 2000-US17380 | 20000622 |
| WO 2000079274 | A3 | 20020110 | | |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

| | | | | |
|---|---|---|---|---|
| US 6323039 | B1 | 20011127 | US 1999-338122 | 19990622 |
| US 6280981 | B1 | 20010828 | US 2000-514569 | 20000223 |
| EP 1210596 | A2 | 20020605 | EP 2000-943119 | 20000622 |

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL

| | | | | |
|---|---|---|---|---|
| JP 2003506014 | T2 | 20030218 | JP 2001-505191 | 20000622 |

PRIORITY APPLN. INFO.: US 1999-140433P P 19990622
US 1999-338122 A 19990622
US 2000-176383P P 20000114
WO 2000-US17380 W 20000622

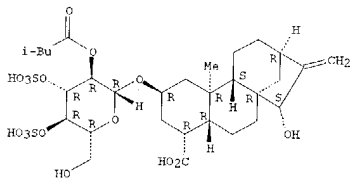
AB The invention provides compns. and methods for monitoring subcellular compartments such as organelles by energy transfer techniques that do not require specific intermol. affinity binding events between energy transfer donor and energy transfer acceptor mols. pH. Provided are methods for assaying cellular membrane potential, including mitochondrial membrane potential, by energy transfer methodologies including fluorescence resonance energy transfer (FRET). Diagnostic and drug screening assays are also provided.

IT **17754-44-8**, Atractyloside **33286-30-5**, Carboxyatractyloside
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(compns. and methods for assaying subcellular conditions and processes using energy transfer for drug screening)

RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

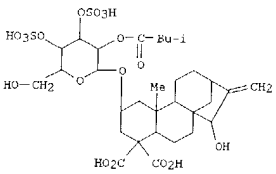
Absolute stereochemistry.

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 K

RN 33286-30-5 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,15α)- (9CI) (CA INDEX NAME)



●2 K

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:314834 CAPLUS
DOCUMENT NUMBER: 132:344104
TITLE: Cloning and production of human adenine nucleotide translocator and the synthesis and screening assays for novel ligands
INVENTOR(S): **Anderson, Christen M.; Davis, Robert E.; Clevenger, William; Wiley, Sandra Eileen; Miller, Scott W.**; Szabo, Tomas R.; **Ghosh, Soumitra S.**
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 175 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000026370 | A2 | 20000511 | WO 1999-US25883 | 19991103 |
| WO 2000026370 | A3 | 20001116 | | |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1049780 | A1 | 20001108 | EP 1999-968032 | 19991103 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| JP 2002539761 | T2 | 20021126 | JP 2000-579742 | 19991103 |
| US 2001044144 | A1 | 20011122 | US 2001-811094 | 20010314 |
| US 2002012992 | A1 | 20020131 | US 2001-810644 | 20010314 |

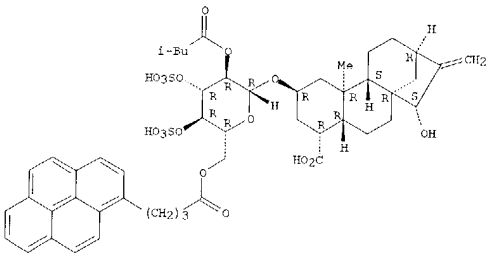
PRIORITY APPLN. INFO.: US 1998-185904 A 19981103
US 1999-393441 A 19990908
WO 1999-US25883 W 19991103

OTHER SOURCE(S): MARPAT 132:344104

AB Compns. and methods are provided for producing adenine nucleotide translocator (ANT) polypeptides and fusion proteins, including the production and use of recombinant expression constructs having a regulated promoter. Bacterial, insect, yeast (Sf9 cells and Trichoplusia ni cells), and mammalian expression systems are designed for reliable production of recombinant human ANT polypeptides in significant quantities, by employing regulated promoters and recombinant ANT fusion products with glutathione S-transferase and green fluorescent protein. The synthesis and properties of representative atractyloside derivs. as ANT ligands are described. ANT ligands and compns. and methods for identifying ANT ligands, agents that bind ANT, and agents that interact with ANT are also disclosed.

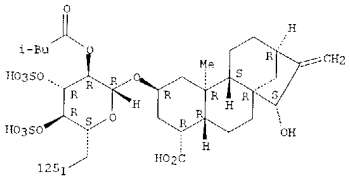
IT **267886-17-9P 267886-18-0P 267886-19-1P**
RL: ARG (Analytical reagent use); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-19-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-deoxy-6-(iodo-125I)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **267886-22-6P 267886-23-7P 267886-24-8P 267886-25-9P 267886-26-0P 267886-27-1P 267886-28-2P 267886-29-3P 267886-30-6P 267886-31-7P 267886-50-0P 267886-51-1P 267886-56-6P 267886-57-7P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(cloning and production of human adenine nucleotide translocator and the synthesis and screening assays for novel ligands)

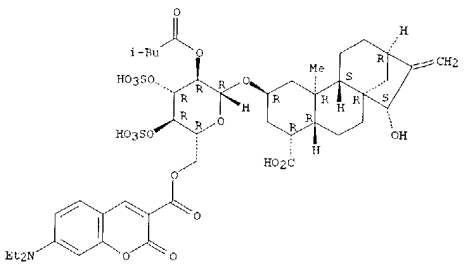
RN 267886-22-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[[[[4-[[[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl](carboxymethyl)amino]methyl]phenyl]amino]thioxomethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(cloning and prodn. of human adenine nucleotide translocator and the synthesis and screening assays for novel ligands)

RN 267886-17-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[[7-(diethylamino)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

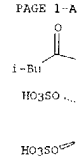


RN 267886-18-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-[1-oxo-4-(1-pyrenyl)butyl]-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

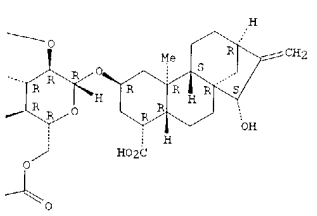
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B



PAGE 2-A

RN 267886-23-7 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-[[[[4-[[[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl](carboxymethyl)amino]methyl]phenyl]amino]thioxomethyl]amino]-6-deoxy-2-O-(3-methyl-1-

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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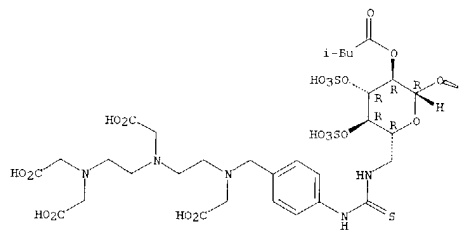
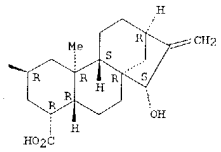


PAGE 1-B

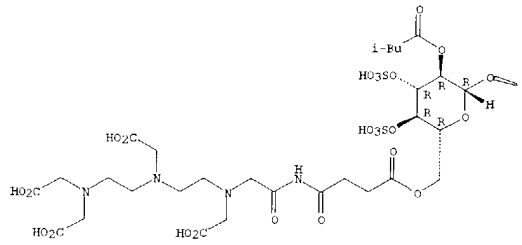


RN 267886-24-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[15-carboxy-8,11,14-tris(carboxymethyl)-1,4,6-trioxo-5,8,11,14-tetraazapentadec-1-yl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

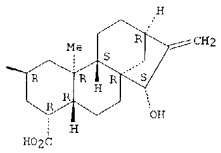
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B

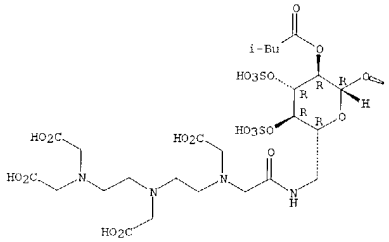


RN 267886-25-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-[[[[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl](carboxymethyl)amino]acetyl]amino]-6-deoxy-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

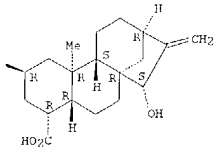
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B



RN 267886-26-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]carbonyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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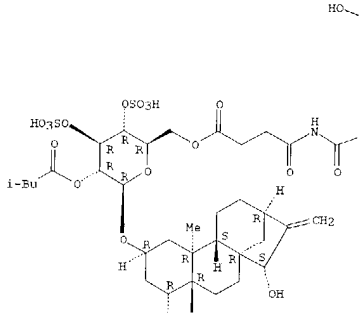
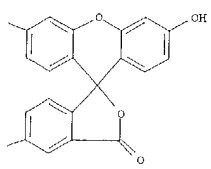


PAGE 1-B



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RN 267886-27-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-deoxy-6-[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]carbonyl]amino]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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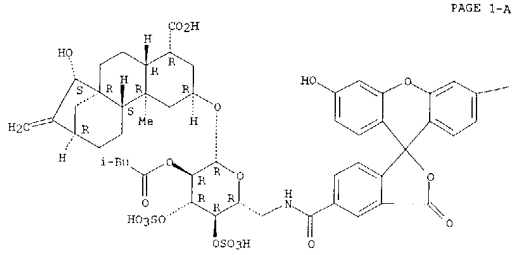

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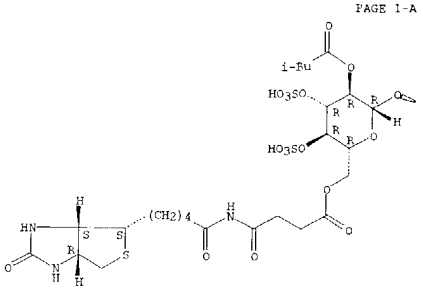
RN 267886-28-2 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

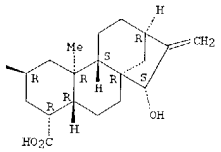
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



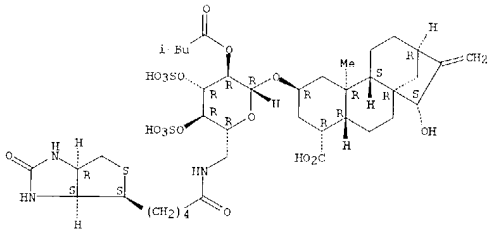
PAGE 1-B



RN 267886-29-3 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-deoxy-6-[[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]amino]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

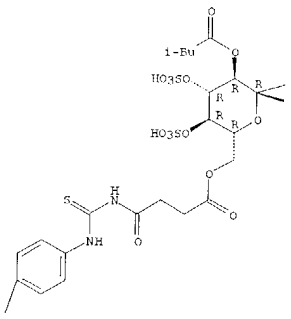
L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-30-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[[[[4-[2-[2,6-bis[3-carboxy-2-(carboxymethyl)propyl]-4-pyridinyl]ethyl]phenyl]amino]thioxomethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

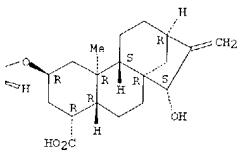
Absolute stereochemistry.

PAGE 1-A

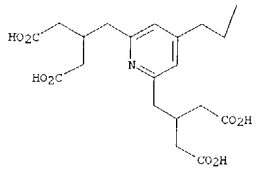


L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-B



PAGE 2-A



RN 267886-31-7 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-[[[[4-[2-[2,6-bis[3-carboxy-2-(carboxymethyl)propyl]-4-pyridinyl]ethyl]phenyl]amino]thioxomethyl]amino]-6-deoxy-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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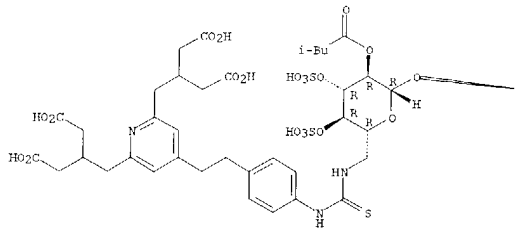

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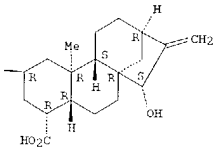

RN 267886-50-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[[(2',7'-difluoro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)carbonyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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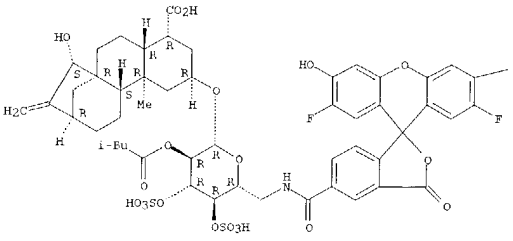

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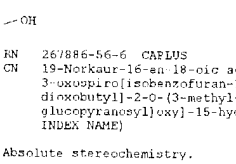

RN 267886-56-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[[(2',7'-dichloro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)carbonyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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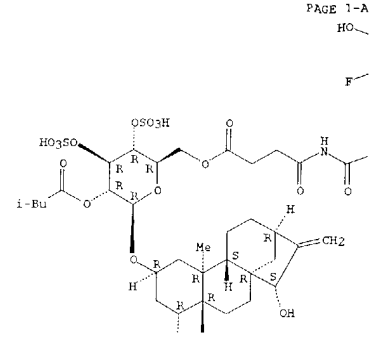

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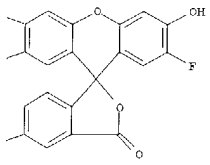

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RN 267886-51-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-deoxy-6-[[(2',7'-difluoro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)carbonyl]amino]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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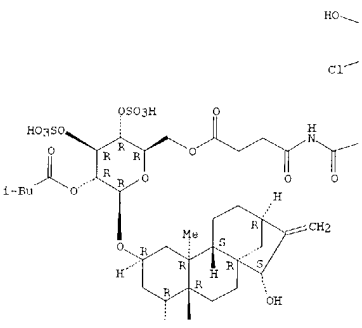

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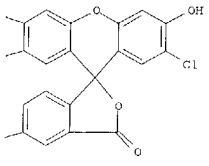

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RN 267886-57-7 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-deoxy-6-[[(2',7'-dichloro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)carbonyl]amino]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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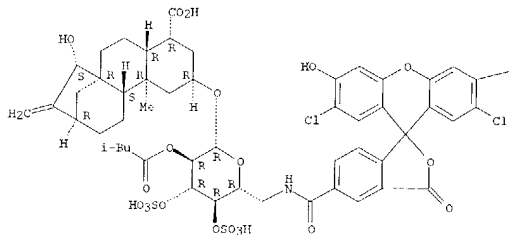

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—OH

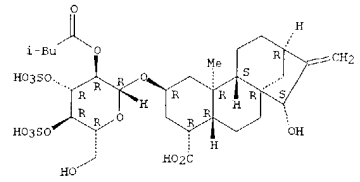
IT **17754-44-8P**, Atractyloside **33286-30-5DP**,
Carboxyatractyloside, derivs. **268557-13-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(cloning and production of human adenine nucleotide translocator and the synthesis and screening assays for novel ligands)

RN 17754-44-8 CAPLUS

CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

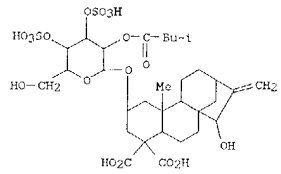
L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 K

RN 33286-30-5 CAPLUS

CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,15α)- (9CI) (CA INDEX NAME)



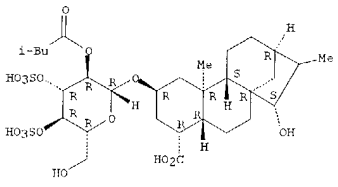
●2 K

RN 268557-13-7 CAPLUS

CN 19-Norkauran-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α,16ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

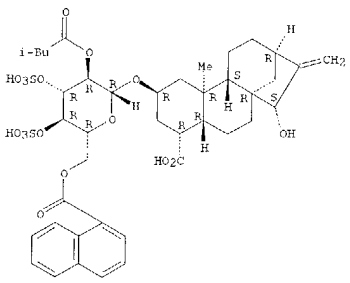


IT **84882-67-7P 267886-32-8P 267886-33-9P**
**267886-34-0P 267886-35-1P 267886-36-2P**
**267886-37-3P 267886-38-4P 267886-39-5P**
**267886-40-8P 267886-41-9P 267886-42-0P**
**267886-43-1P 267886-44-2P 267886-45-3P**
**267886-46-4P 267886-47-5P 267886-48-6P**
**267886-49-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(cloning and production of human adenine nucleotide translocator and the synthesis and screening assays for novel ligands)

RN 84882-67-7 CAPLUS

CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-(1-naphthalenylcarbonyl)-2,3-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 267886-32-8 CAPLUS

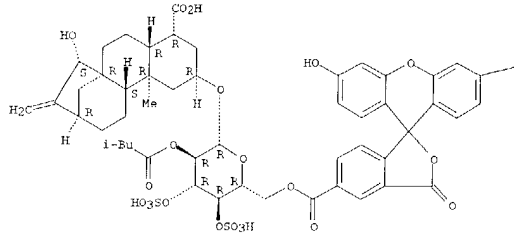
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)carbonyl]-2-O-(3-methyl-

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

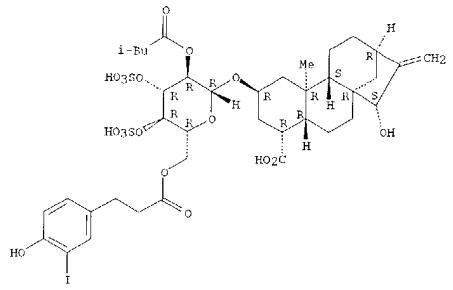
—OH

RN 267886-33-9 CAPLUS

CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxy-3-iodophenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

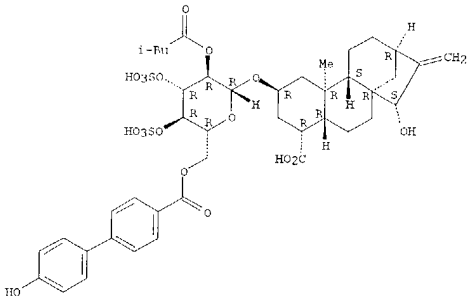
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



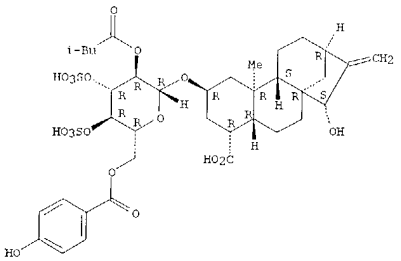
RN 267886-34-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[(4'-hydroxy[1,1'-biphenyl]-4-yl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



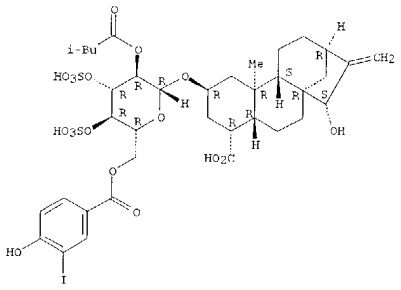
RN 267886-35-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[(4'-hydroxy-3'-iodo[1,1'-biphenyl]-4-yl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-37-3 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-(4-hydroxy-3-iodobenzoyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



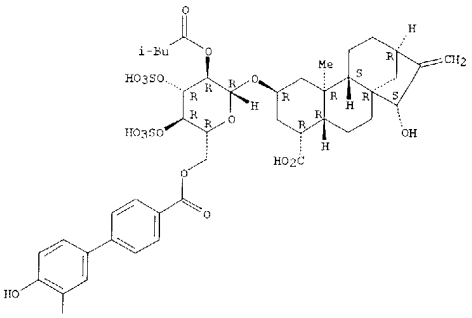
RN 267886-38-4 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[(6-hydroxy-5-iodo-2-naphthalenyl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



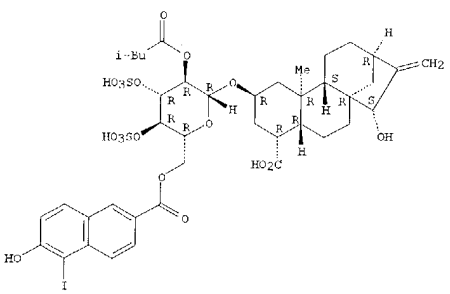
PAGE 2-A



RN 267886-36-2 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-(4-hydroxybenzoyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

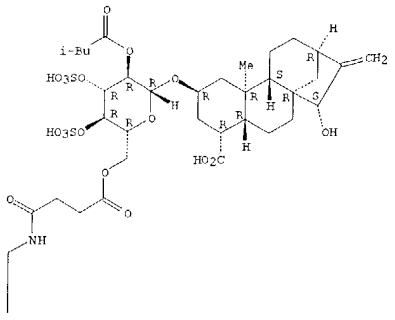
L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-39-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-[[2-(4-hydroxyphenyl)ethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

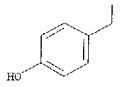
Absolute stereochemistry.

PAGE 1-A



L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

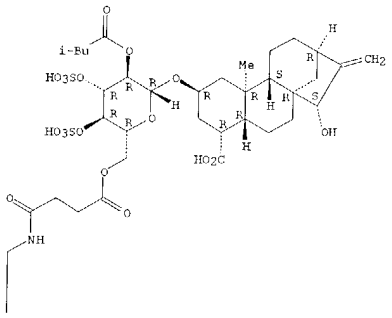
PAGE 2-A



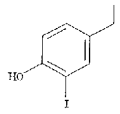
RN 267886-40-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-[[2-(4-hydroxy-3-iodophenyl)ethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

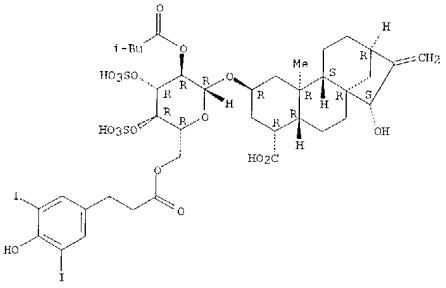
PAGE 1-A



PAGE 2-A

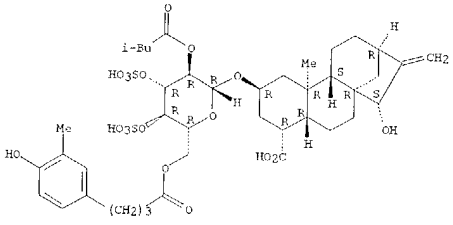


L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-43-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-(4-hydroxy-3-methylphenyl)-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 267886-44-2 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-(4-hydroxy-3-iodo-5-methylphenyl)-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

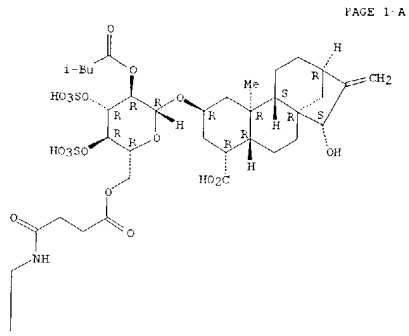
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 267886-41-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-[[2-(4-hydroxy-3,5-diiodophenyl)ethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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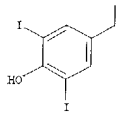
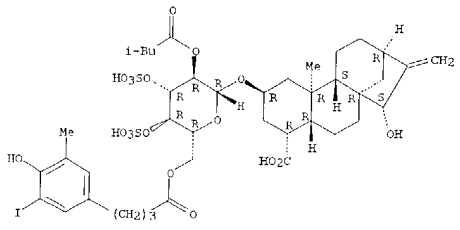


RN 267886-42-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxy-3,5-diiodophenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

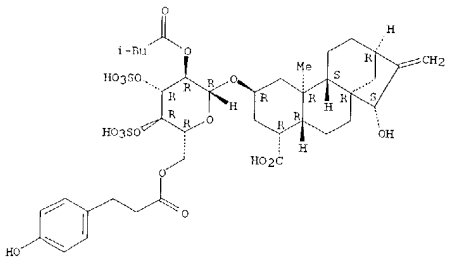
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-45-3 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxyphenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

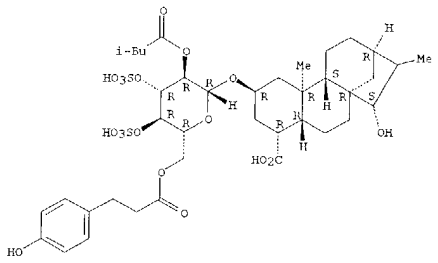
Absolute stereochemistry.



RN 267886-46-4 CAPLUS
CN 19-Norkauran-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxyphenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α,16ξ)- (9CI) (CA INDEX NAME)

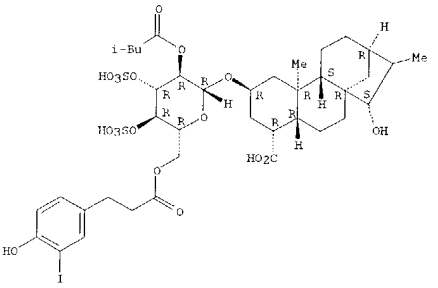
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



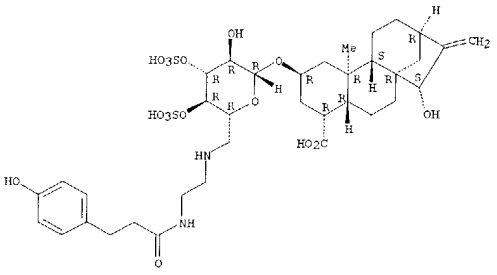
RN 267886-47-5 CAPLUS
CN 19-Norkauran-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxy-3-iodophenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α,16ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



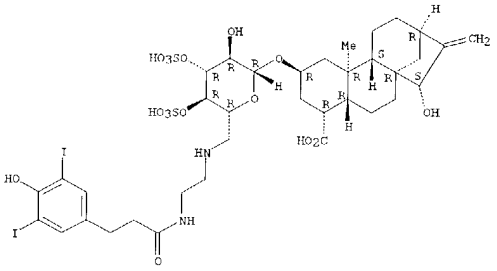
RN 267886-48-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-deoxy-6-[[2-[[3-(4-hydroxyphenyl)-1-oxopropyl]amino]ethyl]amino]-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
Absolute stereochemistry.



RN 267886-49-7 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-deoxy-6-[[2-[[3-(4-hydroxy-3,5-diiodophenyl)-1-oxopropyl]amino]ethyl]amino]-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

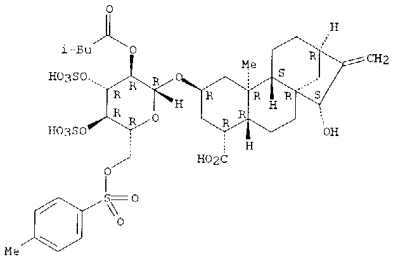
Absolute stereochemistry.



IT **267886-16-8P 267886-20-4P 267886-21-5DP, alkyldiamine derivs. 267886-21-5P 267886-53-3P 267886-55-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cloning and prodn. of human adenine nucleotide translocator and the synthesis and screening assays for novel ligands)

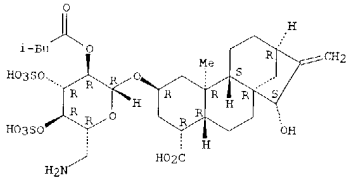
RN 267886-16-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-[(4-methylphenyl)sulfonyl]-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 267886-20-4 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-amino-6-deoxy-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

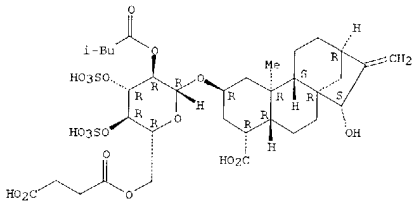
Absolute stereochemistry.



RN 267886-21-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-(3-carboxy-1-oxopropyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

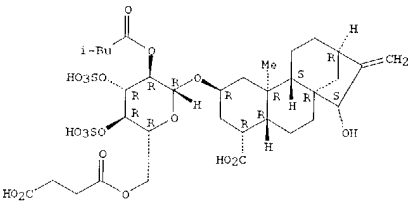
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-21-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-(3-carboxy-1-oxopropyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 267886-53-3 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[(4'-hydroxy-3',5'-diiodo[1,1'-biphenyl]-4-yl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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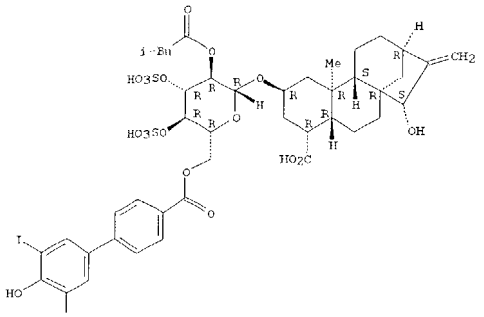

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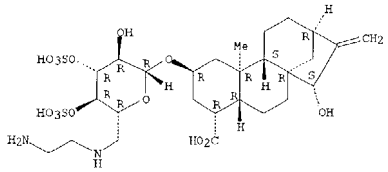
RN 267886-55-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-[(2-aminoethyl)amino]-6-deoxy-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:227858 CAPLUS
DOCUMENT NUMBER: 132:260666
TITLE: Identifying agents that alter mitochondrial permeability transition pores and cell death for diagnostic and therapeutic use
INVENTOR(S): Dykens, James A.; **Miller, Scott W.**; **Ghosh, Soumitra S.**; **Davis, Robert E.**
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000019200 | A1 | 20000406 | WO 1999-US22261 | 19990924 |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 2003044776 | A1 | 20030306 | US 1998-161172 | 19980925 |
| CA 2345066 | AA | 20000406 | CA 1999-2345066 | 19990924 |
| AU 9961628 | A1 | 20000417 | AU 1999-61628 | 19990924 |
| EP 1116027 | A1 | 20010718 | EP 1999-948458 | 19990924 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| JP 2002525630 | T2 | 20020813 | JP 2000-572655 | 19990924 |

PRIORITY APPLN. INFO.: US 1998-161172 A 19980925
WO 1999-US22261 W 19990924

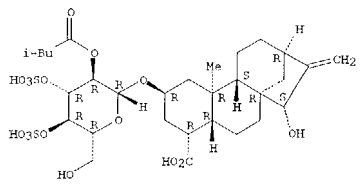
AB Methods are provided for identifying agents that affect mitochondrial functions and cell death. Such agents are useful for treating diseases associated with mitochondrial dysfunction and in methods of identifying a risk or presence of such diseases. In particular, the invention relates to the loss of mitochondrial membrane potential (ΔΨm) during mitochondrial permeability transition (MPT) and further provides a measurable rate loss function, changes in which are useful e.g. for detecting agents that affect one or more mitochondrial functions, for detecting mitochondrial diseases, and for studying mol. components of mitochondria that regulate MPT.

IT **17754-44-8**, Atractyloside
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(identification of agents that alter mitochondrial permeability transition pores and cell death for diagnostic and therapeutic use)

RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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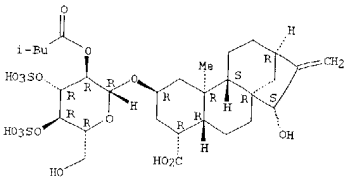
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:206474 CAPLUS
DOCUMENT NUMBER: 100:206474
TITLE: Toxic constituents in Mongolian Xanthium (Xanthium mongolicum) kernel
AUTHOR(S): Wang, Suxian; Ren, Lijuan; Sun, Zeren; **Pei, Yuehu**; Zhu, Tingru
CORPORATE SOURCE: Shenyang Coll. Pharm., Shanyang, Peop. Rep. China
SOURCE: Zhongcaoyao (1983), 14(12), 529-31
CODEN: CTYAD8; ISSN: 0253-2670
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI For diagram(s), see printed CA Issue.
AB A toxic glycoside, atractyloside (I), was isolated from a hot water extract of defatted powdered seeds of X. mongolicum 1st by successive treatment and precipitation with 50% EtOH, 70% acetone, and 10% Pb acetate, followed by filtration; the filtrate was washed with H2S to remove Pb and I was crystallized with 70% EtOH. The structure of I was determined by chemical and spectral methods.
IT **17754-44-8**
RL: BIOL (Biological study)
(of mongolian xanthium kernels)
RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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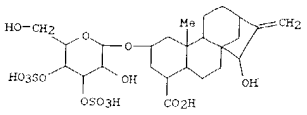
IT **90319-99-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 90319-99-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[3,4-di-O-sulfo-β-D-glucopyranosyl)oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L7 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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L2           12 S L1
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L5           11 S L3 NOT L4

     FILE 'CAPLUS' ENTERED AT 09:04:31 ON 29 MAR 2004
L6          449 S L4
L7            9 S L4 AND (ANDERSON C? OR DAVIS R? OR CLEVENGER W? OR WILEY S? O

=> s l6 and atrectyloside
            0 ATRECTYLOSIDE
L8          0 L6 AND ATRECTYLOSIDE

=> s l6 and ANT
         4723 ANT
         2281 ANTS
         5616 ANT
                (ANT OR ANTS)
L9          9 L6 AND ANT

=> s l9 not l7
L10         7 L9 NOT L7

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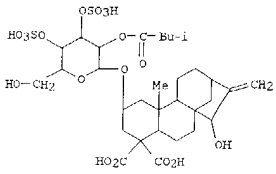
L10 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:371325 CAPLUS
DOCUMENT NUMBER: 139:287714
TITLE: Adenine Nucleotide Translocase Mediates the KATP-Channel-Openers-Induced Proton and Potassium Flux to the Mitochondrial Matrix
AUTHOR(S): Kopustinskiene, Dalia M.; Toleikis, Adolfas; Saris, Nils-Erik L.
CORPORATE SOURCE: Institute for Biomedical Research, Kaunas University of Medicine, Kaunas, LT-3007, Lithuania
SOURCE: Journal of Bioenergetics and Biomembranes (2003), 35(2), 141-148
CODEN: JBIBD4; ISSN: 0145-479X
PUBLISHER: Kluwer Academic/Plenum Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB KATP channel openers have been shown to protect ischemic-reperfused myocardium by mimicking ischemic preconditioning, although their mechanisms of action have not been fully clarified. In this study we investigated the influence of the adenine nucleotide translocase ( **ANT**) inhibitors-carboxyatractyloside (CAT) and bongkrekic acid (BA)-on the diazoxide- and pinacidil-induced uncoupling of isolated rat heart mitochondria respiring on pyruvate and malate (6&6 mM). We found that both CAT (1.3 μM) and BA (20 μM) markedly reduced the uncoupling of mitochondrial oxidative phosphorylation induced by the KATP channel openers. Thus, the uncoupling effect of diazoxide and pinacidil is evident only when **ANT** is not fixed by inhibitors in neither the C- nor the M-conformation. Moreover, the uncoupling effect of diazoxide and pinacidil was diminished in the presence of ADP or ATP, indicating a competition of KATP channel openers with adenine nucleotides. CAT also abolished K+-dependent mitochondrial respiratory changes. Thus **ANT** could also be involved in the regulation of KATP-channel-openers-induced K+ flux through the inner mitochondrial membrane.

IT **33286-30-5**, Carboxyatractyloside
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(adenine nucleotide translocase mediates the KATP-channel-openers-induced proton and potassium flux to the mitochondrial matrix)
RN 33286-30-5 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,15α)- (9CI) (CA INDEX NAME)

L10 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

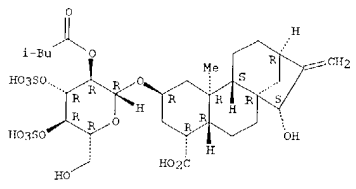
L10 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:669391 CAPLUS
DOCUMENT NUMBER: 139:18447
TITLE: Mitochondrial permeability transition as a novel principle of hepatorenal toxicity in vivo
AUTHOR(S): Haouzi, D.; Cohen, I.; Vieira, H. L. A.; Poncet, D.; Boya, P.; Castedo, M.; Vadrot, N.; Belzacq, A.-S.; Fau, D.; Brenner, C.; Feldmann, G.; Kroemer, G.
CORPORATE SOURCE: Institut Gustave Roussy, Centre National de la Recherche Scientifique, UMR1599, Villejuif, F-94805, Fr.
SOURCE: Apoptosis (2002), 7(5), 395-405
CODEN: APOPFN; ISSN: 1360-8185
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Atractyloside (Atr) binds to the adenine nucleotide translocator ( **ANT**) and inhibits **ANT**-mediated ATP/ADP exchange on the inner mitochondrial membrane. In addition, Atr can trigger opening of a non-specific ion channel, within the **ANT**-containing permeability transition pore complex (PTPC), which is subject to redox regulation and inhibited by cyclosporin A (CsA). The cytotoxic effects of Atr, both in vivo and in vitro, are determined by its capacity to induce PTPC opening and consequent mitochondrial membrane permeabilization (MMP). Thus, the Atr-induced MMP and death of cultured liver cells are both inhibited by CsA as well as by glutathione (GSH) and enhanced by GSH depletion. Similarly, the hepatorenal toxicity of Atr, assessed in vivo, was reduced by treating mice with CsA or a diet rich in sulfur amino acids, a regime which enhances mitochondrial GSH levels. Atr injection induced MMP in hepatocytes and proximal renal tubular cells, and MMP was reduced by either CsA or GSH. Acetaminophen (paracetamol)-induced acute poisoning was also attenuated by CsA and GSH, both in vitro and in vivo. Altogether these data indicate that PTPC-mediated MMP may determine the hepatorenal toxicity of xenobiotics in vivo.

IT **17754-44-8**, Atractyloside
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(mitochondrial permeability transition as novel principle of hepatorenal toxicity in mice following atractyloside and acetaminophen administration)
RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4a,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

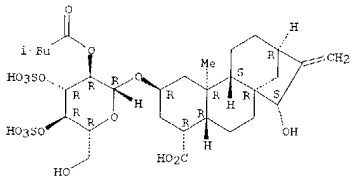
L10 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:394447 CAPLUS
DOCUMENT NUMBER: 137:137553
TITLE: Pyrophosphate import and synthesis by plant mitochondria
AUTHOR(S): Casolo, Valentino; Micolini, Stefano; Macri, Francesco; Vianello, Angelo
CORPORATE SOURCE: Department of Biology and Agro-industrial Economics, Section of Plant Biology, University of Udine, Udine, I-33100, Italy
SOURCE: Physiologia Plantarum (2002), 114(4), 516-523
CODEN: PHPLAI; ISSN: 0031-9317
PUBLISHER: Blackwell Munksgaard
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The matrix level of pyrophosphate (PPi) in mitochondria isolated from etiolated pea (Pisum sativum L. cv. Alaska) stems was evaluated, on the basis of an enzymic assay, to be approx. 0.2 mM. Pyrophosphate could enter from the cytoplasm to the mitochondria via adenine nucleotide translocase (**ANT**), because F- and Ca2- (two penetrating PPiase inhibitors) and atractylate (**ANT** inhibitor) inhibited PPiase activity in isolated mitochondria supplied with PPi. This result was also confirmed by measuring oxygen consumption and membrane potential (Δψ) in succinate-energized mitochondria. In a medium free of phosphate (Pi), the addition of PPi before the substrate rendered possible an ADP-stimulated oxygen consumption that was inhibited by F- or Ca2+. In a similar experiment, ADP induced the dissipation of Δψ when it was added after the succinate-generated Δψ had reached a steady state and, again, F inhibited this dissipation. These results imply that PPi enters the mitochondria where it is hydrolyzed to 2 Pi which become available for the H+-ATPase (EC 3.6.1.34). In addition, PPi may be synthesized by the H+-PPiase (EC 3.6.1.1), acting as a synthase. This evidence arises from the observation that Pi stimulated an oxygen consumption (respiratory control ratio of 1.7) that was inhibited by F- or Ca2-. The physiol. role of the mitochondrial H+-PPiase is discussed in the light of the consideration that this enzyme can catalyze a readily reversible reaction.

IT **1398-13-6**
RL: BSU (Biological study, unclassified); BIOL (Biological study) (pyrophosphate import and synthesis by plant mitochondria)
RN 1398-13-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:185165 CAPLUS
DOCUMENT NUMBER: 136:243571
TITLE: Mechanism of mitochondrial membrane permeabilization by HIV-1 Vpr, mimetics of Vpr and methods of screening active molecules having the ability to alter and/or prevent and/or mimic the interaction of Vpr with **ANT**
INVENTOR(S): Jacotot, Etienne Daniel Francois; Kroemer, Guido; Roques, Bernard Pierre; Edelmann, Lena; Hoebeke, Johan; Brenner-Jan, Catherine; Belzacq, Anne-Sophie
PATENT ASSIGNEE(S): Institut Pasteur, Fr.; Centre National de la Recherche Scientifique; Institut National de la Sante et de la Recherche Medicale - INSERM; Universite de Technologie de Compiegne
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2002020570 | A2 | 20020314 | WO 2001-EP11316 | 20010911 |
| WO 2002020570 | A3 | 20031002 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2002015004 | A5 | 20020322 | AU 2002 15004 | 20010911 |
| EP 1370572 | A2 | 20031217 | EP 2001-983518 | 20010911 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| JP 2004508385 | T2 | 20040318 | JP 2002-525189 | 20010911 |
| US 2002068273 | A1 | 20020606 | US 2001-949650 | 20010912 |

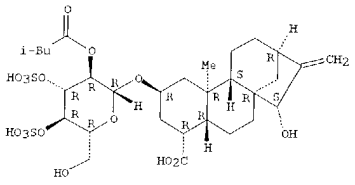
PRIORITY APPLN. INFO.: US 2000-231539P P 20000911
US 2000-232841P P 20000915
WO 2001-EP11316 W 20010911

AB The invention is directed to the induction of mitochondrial membrane permeabilization via the phys. and functional interaction of the HIV-1 proapoptotic Vpr protein with the mitochondrial inner membrane protein **ANT** (adenine nucleotide translocator, also called adenine nucleotide translocase or ADP/ATP carrier). HIV-1 Vpr (viral protein R) interacts with the permeability transition pore complex (PTPC) to trigger **ANT** pore formation and/or mitochondrial membrane permeabilization and consequent cell death. Reagents and methods fo inducing and/or inhibiting the binding of Vpr to **ANT**, mitochondrial membrane permeabilization, and apoptosis are provided.

IT **17754-44-8**, Atractyloside
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(mechanism of mitochondrial membrane permeabilization by HIV-1 Vpr, mimetics of Vpr and methods of screening active mols. altering, preventing or mimicking interaction of Vpr with **ANT**)
RN 17754-44-8 CAPLUS

L10 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 X

L10 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:150868 CAPLUS
DOCUMENT NUMBER: 137:337
TITLE: Cytochrome c oxidase subunit III. A molecular marker for n-(4-hydroxyphenyl)retinamide-induced oxidative stress in hepatoma cells
AUTHOR(S): You, Kyung-Ran; Wen, Jing; Lee, Soo-Taek; Kim, Dae-Ghon
CORPORATE SOURCE: Division of Gastroenterology and Hepatology, Department of Internal Medicine, Institute for Molecular Biology and Genetics, Chonbuk National University Medical School and Hospital, Jeonju, 561-712, S. Korea
SOURCE: Journal of Biological Chemistry (2002), 277(6), 3870-3877
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

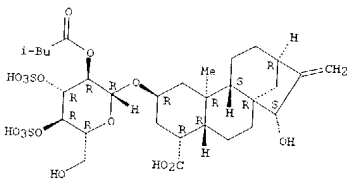
AB N-(4-hydroxyphenyl)retinamide (4HPR), a chemopreventive and chemotherapeutic retinoid, induces apoptosis in various types of cells. Currently, oxidative mitochondrial damage is thought to cause 4HPR-induced apoptosis, although the exact mechanism has not yet been clarified. 4HPR effectively induces apoptosis in hepatoma cells although the susceptibility differs in a cell-specific manner. Hep-3B and PLC/PRF/5 cells were more susceptible to 4HPR than were Hep-G2 and SKHEP-1 cells, and the resistance to 4HPR seems to be related to growth inhibition (G1 arrest). We further observed that 4HPR specifically down-regulates cytochrome c oxidase subunit III (CO III) transcript levels through destabilization of its mRNA and thus decreases the activity of cytochrome c oxidase (complex IV). To explore the mechanism whereby the CO III transcript was decreased by 4HPR, we used adenine nucleotide translocator (**ANT**) ligands, which modulate mitochondrial transmembrane potential (Δψm) without altering CO III transcription. Intriguingly, bongkrekic acid, a specific **ANT** inhibitor, enhanced 4HPR-induced Δψm disruption, which in turn decreased the level of CO III transcripts, which was accompanied by increases in the generation of reactive oxygen species and in apoptosis. In contrast, atractyloside, an activator of **ANT**, inhibited those 4HPR-induced effects. Taken together, these results indicate that down-regulation of CO III, a mol. marker of oxidative stress, may result from upstream Δψm disruption and that ligands of **ANT** may be capable of modulating 4HPR-induced oxidative stress and apoptosis.

IT **17754-44-8**, Atractyloside
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(mechanism of (hydroxyphenyl)retinamide-induced oxidative stress and apoptosis in hepatoma)

RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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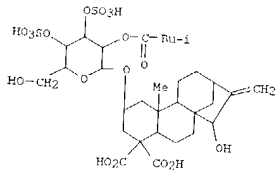
REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:525529 CAPLUS
DOCUMENT NUMBER: 133:248479
TITLE: Copper sensitizes the mitochondrial permeability transition to carboxyatractyloside and oleate
AUTHOR(S): Garcia, Noemi; Zazueta, Cecilia; Carrillo, Raymundo; Correa, Francisco; Chavez, Edmundo
CORPORATE SOURCE: Departamento de Bioquimica, Instituto Nacional de Cardiologia, 014080, Mex.
SOURCE: Molecular and Cellular Biochemistry (2000), 209(1&2), 119-123
CODEN: MCRIB8; ISSN: 0300-8177
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Addition of 5 μM copper to rat kidney mitochondria enhances the effect of carboxyatractyloside and oleate on pore opening, in a cyclosporin A-sensitive fashion. The effects of the pair copper-carboxyatractyloside were observed on matrix Ca2+ efflux, mitochondrial swelling and on the transmembrane elec. gradient. The effect of Cu2+ emphasizes the importance of membrane thiol groups located, probably, in the ADP/ATP translocase (**ANT**), on permeability transition. It was also found that Cu2+ does not block the fluorescent label of **ANT** by eosin 5-maleimide, but abolishes the inhibition by CAT on the labeling. This suggests that the binding of Cu2+ to cysteine residues of **ANT** promotes a conformational change in the carrier, strengthening the effect of CAT and oleate on membrane leakage.

IT **33286-30-5**, Carboxyatractyloside
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(copper sensitizes the mitochondrial permeability transition to carboxyatractyloside and oleate)

RN 33286-30-5 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,15α)- (9CI) (CA INDEX NAME)



●2 K

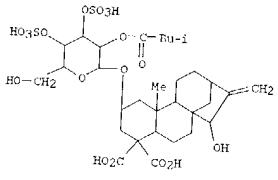
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:475395 CAPLUS
DOCUMENT NUMBER: 113:75395
TITLE: Does the function of adenine nucleotide translocase in fatty acid uncoupling depend on the type of mitochrondria?
AUTHOR(S): Schoenfeld, Peter
CORPORATE SOURCE: Inst. Biochem., Med. Akademie Magdeburg, Magdeburg, 3090, Ger. Dem. Rep.
SOURCE: FEBS Letters (1990), 264(2), 246-8
CODEN: FEBLAL; ISSN: 0014-5793
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The stimulation of respiration by long-chain fatty acids and FCCP was studied with oligomycin-inhibited mitochondria from rat liver, heart, and kidney (RLM, RHM, and RKM, resp.) tissue. By addition of equal amts. of palmitate and oleate, mitochondrial respiration was increased in the order RLM < RKM < RHM. Using the classical photonophore FCCP, this difference could not be observed Inhibition of oleate-stimulated respiration by carboxyatractyloside (CAT) decreased in the order RHM > RKM > RLM. As CAT sensitivity of oleate-stimulated respiration and the mitochondrial adenine nucleotide translocase (**ANT**) content were found to be correlated, it is suggested that the weak CAT sensitivity of oleate-stimulated respiration of RLM is due to the low content of **ANT**.

IT **33286-30-5**, Carboxyatractyloside
RL: BIOL (Biological study)
(oleate-stimulated respiration by mitochondria inhibition by, adenine nucleotide translocase content in relation to)

RN 33286-30-5 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,15α)- (9CI) (CA INDEX NAME)



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=> s l6 and (Alzheimer or Alzheimers or Alzheimer's)
MISMATCHED QUOTE 'ALZHEIMER'S'
Quotation marks (or apostrophes) must be used in pairs,
one before and one after the expression you are setting
off or masking.

=> s l6 and (Alzheimer or Alzheimers)
         29320 ALZHEIMER
          2190 ALZHEIMERS
         29364 ALZHEIMER
                 (ALZHEIMER OR ALZHEIMERS)
          2190 ALZHEIMERS
L11          3 L6 AND (ALZHEIMER OR ALZHEIMERS)

=> d his

     (FILE 'HOME' ENTERED AT 09:02:25 ON 29 MAR 2004)

     FILE 'REGISTRY' ENTERED AT 09:02:32 ON 29 MAR 2004
L1               STRUCTURE UPLOADED
L2            12 S L1
L3           179 S L1 FULL
L4           168 S L3 AND CAPLUS/LC
L5            11 S L3 NOT L4

     FILE 'CAPLUS' ENTERED AT 09:04:31 ON 29 MAR 2004
L6           449 S L4
L7             9 S L4 AND (ANDERSON C? OR DAVIS R? OR CLEVENGER W? OR WILEY S? O
L8             0 S L6 AND ATRECTYLOSIDE
L9             9 S L6 AND ANT
L10            7 S L9 NOT L7
L11            3 S L6 AND (ALZHEIMER OR ALZHEIMERS)

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=> s l11 not l10
L13            3 L11 NOT L10

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L13 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:406465 CAPLUS
DOCUMENT NUMBER: 137:197709
TITLE: High-throughput assessment of mitochondrial membrane potential in situ using fluorescence resonance energy transfer
AUTHOR(S): Dykens, James A.; Fleck, Beth; Ghosh, Soumitra; Lewis, Michelle; Velicelebi, Gonul; Ward, Manus W.
CORPORATE SOURCE: MitoKor, San Diego, CA, 92121, USA
SOURCE: Mitochondrion (2002), 1(5), 461-473
CODEN: MITOCN; ISSN: 1567-7249
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

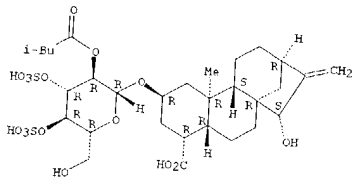
AB Mitochondrial dysfunction causes dozens of debilitating diseases, and is implicated in the etiol. of type 2 diabetes, Parkinson's, and **Alzheimer**'s diseases, among others. However, development of mitochondrially targeted therapeutic agents has been impeded by the lack of high-throughput screening techniques that are capable of distinguishing in intact cells the mitochondrial membrane potential (ΔΨm) from the plasma membrane potential, (ΔΨp). We report here a fluorescence resonance energy transfer (FRET) assay that specifically monitors ΔΨm that is not confounded by background signal arising from potentiometric dye responding to ΔΨp. The technique relies on energy transfer between nonyl acridine orange (NAO), which stains diphosphatidyl glycerol (cardiolipin) that is indigenous to the inner mitochondrial membrane, and tetramethylrhodamine Me ester (TMR), a potentiometric dye that is sequestered by mitochondria as a Nernstian function of ΔΨm and concentration. FRET occurs only when both dyes co-localize to the mitochondria, and results in quenching of NAO emission by TMR in proportion to ΔΨm. Validation studies using compds. with well-characterized mitochondrial effects, including oligomycin, CCCP, nongkrekic acid, cyclosporin A, nigericin, ADP, and ruthenium red, demonstrate that the FRET-based ΔΨm assay responds in accord with the known pharmacol. Validation studies assessing the suitability of the technique for high-throughput compound screening indicate that the assay provides a sensitive and robust assessment not only of mitochondrial integrity in situ, but also, when used in conjunction with agents such as cyclosporin A, an indicator of permeability transition.

IT **17754-44-8**, Atractyloside
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(high-throughput assessment of mitochondrial membrane potential in situ using fluorescence resonance energy transfer)

RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L13 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:911534 CAPLUS
DOCUMENT NUMBER: 134:66121
TITLE: Compositions and methods for assaying subcellular conditions and processes using energy transfer for drug screening
INVENTOR(S): Dykens, James A.; Velicelebi, Gonul; Ghosh, Soumitra S.
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 189 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000079274 | A2 | 20001228 | WO 2000-US17380 | 20000622 |
| WO 2000079274 | A3 | 20020110 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 6323039 | B1 | 20011127 | US 1999-338122 | 19990622 |
| US 6280981 | B1 | 20010828 | US 2000-514569 | 20000223 |
| EP 1210596 | A2 | 20020605 | EP 2000-943119 | 20000622 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | | |
| JP 2003506014 | T2 | 20030218 | JP 2001-505191 | 20000622 |
| PRIORITY APPLN. INFO.: | | | US 1999-140433P P | 19990622 |
| | | | US 1999-338122 A | 19990622 |
| | | | US 2000-176383P P | 20000114 |
| | | | WO 2000-US17380 W | 20000622 |

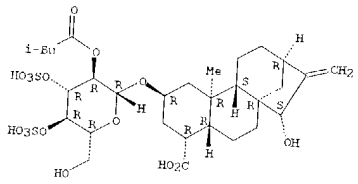
AB The invention provides compns. and methods for monitoring subcellular compartments such as organelles by energy transfer techniques that do not require specific intermol. affinity binding events between energy transfer donor and energy transfer acceptor mols. pH. Provided are methods for assaying cellular membrane potential, including mitochondrial membrane potential, by energy transfer methodologies including fluorescence resonance energy transfer (FRET). Diagnostic and drug screening assays are also provided.

IT **17754-44-8**, Atractyloside **33286-30-5**, Carboxyatractyloside
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(compns. and methods for assaying subcellular conditions and processes using energy transfer for drug screening)

RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L13 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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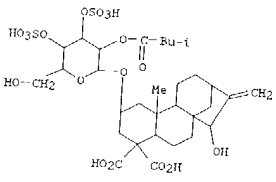
RN 33286-30-5 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,15α)- (9CI) (CA INDEX NAME)



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L13 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:227858 CAPLUS
DOCUMENT NUMBER: 132:260666
TITLE: Identifying agents that alter mitochondrial permeability transition pores and cell death for diagnostic and therapeutic use
INVENTOR(S): Dykens, James A.; Miller, Scott W.; Ghosh, Soumitra S.; Davis, Robert E.
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000019200 | A1 | 20000406 | WO 1999-US22261 | 19990924 |
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| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 2003044776 | A1 | 20030306 | US 1998-161172 | 19980925 |
| CA 2345066 | AA | 20000406 | CA 1999-2345066 | 19990924 |
| AU 9961628 | A1 | 20000417 | AU 1999-61628 | 19990924 |
| EP 1116027 | A1 | 20010718 | EP 1999-948458 | 19990924 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| JP 2002525630 | T2 | 20020813 | JP 2000-572655 | 19990924 |

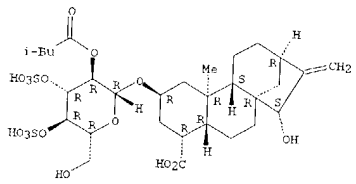
PRIORITY APPLN. INFO.: US 1998-161172 A 19980925
WO 1999-US22261 W 19990924

AB Methods are provided for identifying agents that affect mitochondrial functions and cell death. Such agents are useful for treating diseases associated with mitochondrial dysfunction and in methods of identifying a risk or presence of such diseases. In particular, the invention relates to the loss of mitochondrial membrane potential (ΔΨm) during mitochondrial permeability transition (MPT) and further provides a measurable rate loss function, changes in which are useful e.g. for detecting agents that affect one or more mitochondrial functions, for detecting mitochondrial diseases, and for studying mol. components of mitochondria that regulate MPT.

IT **17754-44-8**, Atractyloside
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(identification of agents that alter mitochondrial permeability transition pores and cell death for diagnostic and therapeutic use)

RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L13 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
Absolute stereochemistry.

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REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> d his

     (FILE 'HOME' ENTERED AT 09:02:25 ON 29 MAR 2004)

     FILE 'REGISTRY' ENTERED AT 09:02:32 ON 29 MAR 2004
L1                STRUCTURE UPLOADED
L2            12 S L1
L3           179 S L1 FULL
L4           168 S L3 AND CAPLUS/LC
L5            11 S L3 NOT L4

     FILE 'CAPLUS' ENTERED AT 09:04:31 ON 29 MAR 2004
L6           449 S L4
L7             9 S L4 AND (ANDERSON C? OR DAVIS R? OR CLEVENGER W? OR WILEY S? O
L8             0 S L6 AND ATRECTYLOSIDE
L9             9 S L6 AND ANT
L10            7 S L9 NOT L7
L11            3 S L6 AND (ALZHEIMER OR ALZHEIMERS)
L12            3 S L11 NOT L9
L13            3 S L11 NOT L10
L14           25 S L6 AND LIGAND

=> s l14 not l9
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=> s l14 not l7
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=> s l16 not l15
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=> d ibib abs hitstr
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L17 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:150868 CAPLUS
DOCUMENT NUMBER: 137:337
TITLE: Cytochrome c oxidase subunit III. A molecular marker for n-(4-hydroxyphenyl)retinamide-induced oxidative stress in hepatoma cells
AUTHOR(S): You, Kyung-Ran; Wen, Jing; Lee, Soo-Taek; Kim, Dae-Ghon
CORPORATE SOURCE: Division of Gastroenterology and Hepatology, Department of Internal Medicine, Institute for Molecular Biology and Genetics, Chonbuk National University Medical School and Hospital, Jeonju, 561-712, S. Korea
SOURCE: Journal of Biological Chemistry (2002), 277(6), 3870-3877
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

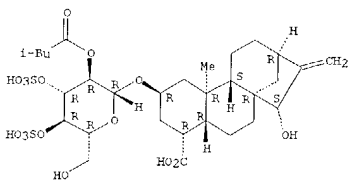
AB N-(4-hydroxyphenyl)retinamide (4HPR), a chemopreventive and chemotherapeutic retinoid, induces apoptosis in various types of cells. Currently, oxidative mitochondrial damage is thought to cause 4HPR-induced apoptosis, although the exact mechanism has not yet been clarified. 4HPR effectively induces apoptosis in hepatoma cells although the susceptibility differs in a cell-specific manner. Hep-3B and PLC/PRF/5 cells were more susceptible to 4HPR than were Hep-G2 and SKHEP-1 cells, and the resistance to 4HPR seems to be related to growth inhibition (G1 arrest). We further observed that 4HPR specifically down-regulates cytochrome c oxidase subunit III (CO III) transcript levels through destabilization of its mRNA and thus decreases the activity of cytochrome c oxidase (complex IV). To explore the mechanism whereby the CO III transcript was decreased by 4HPR, we used adenine nucleotide translocator (ANT) **ligands**, which modulate mitochondrial transmembrane potential (Δψm) without altering CO III transcription. Intriguingly, bongkrekic acid, a specific ANT inhibitor, enhanced 4HPR-induced Δψm disruption, which in turn decreased the level of CO III transcripts, which was accompanied by increases in the generation of reactive oxygen species and in apoptosis. In contrast, atractyloside, an activator of ANT, inhibited those 4HPR-induced effects. Taken together, these results indicate that down-regulation of CO III, a mol. marker of oxidative stress, may result from upstream Δψm disruption and that **ligands** of ANT may be capable of modulating 4HPR-induced oxidative stress and apoptosis.

IT **17754-44-8**, Atractyloside
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(mechanism of (hydroxyphenyl)retinamide-induced oxidative stress and apoptosis in hepatoma)

RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L17 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L15 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:465960 CAPLUS
DOCUMENT NUMBER: 137:47439
TITLE: Preparation of amino acid derivatives for altering mitochondrial function and cellular responses
INVENTOR(S): Pei, Yazhong; Moos, Walter H.; Ghosh, Soumitra S.
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2002048092 | A2 | 20020620 | WO 2001-US48068 | 20011214 |
| WO 2002048092 | A3 | 20030109 | | |
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| AU 2002039595 | A5 | 20020624 | AU 2002-39595 | 20011214 |
| US 2002173543 | A1 | 20021121 | US 2001-20090 | 20011214 |
| US 6552076 | B2 | 20030422 | | |

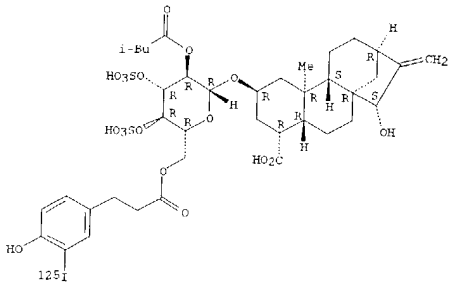
PRIORITY APPLN. INFO.: US 2000-255803P P 20001215
WO 2001-US48068 W 20011214
OTHER SOURCE(S): MARPAT 137:47439

AB Compds. R1COCHR2N(CH2CO2H)CO-A-C6H4NHCOR3 [A is a direct bond, (un)substituted alkyldiyl, -O-(alkyldiyl)-, (alkyldiyl)-O-, -N(R')-(alkyldiyl)- (R' = H or alkyl), (alkyldiyl)-N(R')-, heterocycledlyl, or heterocyclealkyldiyl; R1 = OH, alkoxy, aryloxy, arylalkyloxy, amino, or mono- or dialkylamino; R2 = H, (un)substituted alkyl, aryl, arylalkyl, heterocyclyl, or heterocyclylalkyl; R3 = (un)substituted alkyl, aryl, arylalkyl, heterocyclyl, or heterocyclylalkyl] were prepared for treating diseases by altering mitochondrial function that affects cellular processes. Thus, (HO2CCH2)2NCOC6H4NHAc-o was prepared by substitution reaction of glycine tert-Bu ester acetate with bromoacetate resin, reaction with 2-nitrobenzoic acid, nitro group reduction, acetylation with Ac2O, and resin cleavage using TFA. Biol. activities of compds. of the invention were examined in neuronal viability, displacement of an adenine nucleotide translocase **ligand** from isolated mitochondria, and chondrocyte cytodeprotection assays.

IT **437992-74-0**
RL: BSU (Biological study, unclassified); BIOL (Biological study) (radioligand; measurement of binding efficacy of amino acid derivs. in relation to mitochondrial function and cellular responses)

RN 437992-74-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-[4-hydroxy-3-(iodo-125I)phenyl]-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L15 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

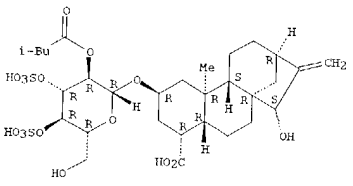
L15 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:832891 CAPLUS
DOCUMENT NUMBER: 136:100280
TITLE: Vaccinia virus infection disarms the mitochondrion-mediated pathway of the apoptotic cascade by modulating the permeability transition pore
AUTHOR(S): Wasilenko, Shawn T.; Meyers, Adrienne F. A.; Vander Helm, Kathleen; Barry, Michele
CORPORATE SOURCE: Department of Medical Microbiology and Immunology, University of Alberta, Edmonton, AB, T6G 2S2, Can.
SOURCE: Journal of Virology (2001), 75(23), 11437-11448
CODEN: JOVIAM; ISSN: 0022-538X
PUBLISHER: American Society for Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Many viruses have evolved strategies that target crucial components within the apoptotic cascade. One of the best studied is the caspase 8 inhibitor, crmA/Spi-2, encoded by members of the poxvirus family. Since many proapoptotic stimuli induce apoptosis through a mitochondrion-dependent, caspase 8-independent pathway, we hypothesized that vaccinia virus would encode a mechanism to directly modulate the mitochondrial apoptotic pathway. In support of this, we observed that Jurkat cells, which undergo Fas-mediated apoptosis exclusively through the mitochondrial route, were resistant to Fas-induced death following infection with a crmA/Spi-2-deficient strain of vaccinia virus. In addition, vaccinia virus-infected cells subjected to the proapoptotic stimulus staurosporine exhibited decreased levels of both cytochrome c released from the mitochondria and caspase 3 activation. In all cases we found that the loss of the mitochondrial membrane potential, which occurs as a result of opening the multimeric permeability transition pore complex, was prevented in vaccinia virus-infected cells. Moreover, vaccinia virus infection specifically inhibited opening of the permeability transition pore following treatment with the permeability transition pore **ligand** atractyloside and t-butylhydroperoxide. These studies indicate that vaccinia virus infection directly impacts the mitochondrial apoptotic cascade by influencing the permeability transition pore.

IT **17754-44-8**, Atractyloside
RL: BSU (Biological study, unclassified); BIOL (Biological study) (vaccinia virus infection disarms mitochondrion-mediated pathway of apoptotic cascade by modulating permeability transition pore)

RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L15 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:168189 CAPLUS
DOCUMENT NUMBER: 134:219377
TITLE: Methods for assaying mitochondrial intermembrane space protein translocation and drug screening
INVENTOR(S): Murphy, Anne N.; Wiley, Sandra Eileen; Andreyev, Alexander Y.
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 70 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001016373 | A2 | 20010308 | WO 2000-US23638 | 20000828 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 1999-151231P P 19990827
US 1999-169508P P 19991207
US 2000-606370 A 20000628

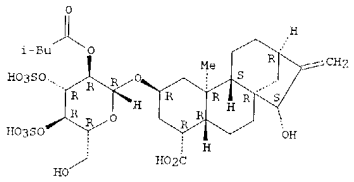
AB Compns. and methods are provided for identifying agents that alter mitochondrial intermembrane space protein (MISP) translocation. The screening methods generally detect agents that alter the level of detectable extramitochondrial MISP following exposure of a cell to an agent known or suspected to induce mitochondrial intermembrane space protein translocation. Such agents may be used, for example, in the treatment of a variety of conditions associated with altered mitochondrial function. SH-SY5Y neuroblastoma cells were transfected with a recombinant expression construct encoding adenylate kinase-2 fusion protein with hemagglutinin epitope tag. Several stable cell lines were established that overexpress the fusion protein. The cells were treated with various apoptogens, harvested, and analyzed by Western blot for cytochrome c and adenylate kinase release from the mitochondria.

IT **17754-44-8**, Atractyloside **33286-30-5**, Carboxyatractyloside
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(methods for assaying mitochondrial intermembrane space protein translocation and drug screening)

RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L15 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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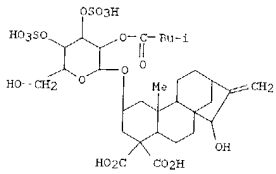
RN 33286-30-5 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,15α)- (9CI) (CA INDEX NAME)



●2 K

L15 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:31673 CAPLUS
DOCUMENT NUMBER: 134:80828
TITLE: Screening method for compds. modulating an AMP-sensitive regulatory site on mitochondria, and use of identified compounds in the treatment of body weight disorders
INVENTOR(S): Brand, Martin Dene; Cadenas, Susana; Dickinson, Keith; Jones, Robert Brian
PATENT ASSIGNEE(S): Knoll Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001002598 | A2 | 20010111 | WO 2000-EP5863 | 20000623 |
| WO 2001002598 | A3 | 20010531 | | |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

| | | | | |
|---|---|---|---|---|
| EP 1214593 | A2 | 20020619 | EP 2000-951299 | 20000623 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | | |
| JP 2003504035 | T2 | 20030204 | JP 2001-508369 | 20000623 |

PRIORITY APPLN. INFO.: GB 1999-15225 A 19990630
GB 1999-15226 A 19990630
GB 2000-4629 A 20000229
WO 2000-EP5863 W 20000623

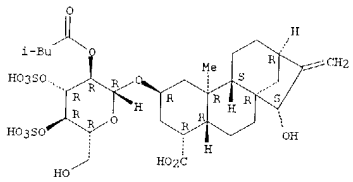
AB The invention provides a screening method for the identification of compds. which modulate an AMP-sensitive regulatory site on mitochondria, comprising (a) contacting a test compound with mitochondria in the presence of a substrate for respiration in the presence of a buffer system; (b) measuring an index of metabolic rate; and (c) identifying compds. which modulate metabolic rate. Alternatively or addnl., membrane potential can be measured. The invention also comprises a regulatory site for a mitochondrial proton leak which is related to the adenine nucleotide carrier, a binding assay and a functional assay. Identified compds. can be used for the treatment of body weight disorders, e.g. obesity and cachexia.

IT **1398-13-6D**, fluorescently labeled
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(screening method for compds. modulating AMP-sensitive regulatory site on mitochondria, and use of compds. for treatment of body weight disorders)

RN 1398-13-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L15 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L15 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:800820 CAPLUS
DOCUMENT NUMBER: 130:164710
TITLE: Binding of Nucleotides by the Mitochondrial ADP/ATP Carrier as Studied by 1H Nuclear Magnetic Resonance Spectroscopy
AUTHOR(S): Huber, Thomas; Klingenberg, Martin; Beyer, Klaus
CORPORATE SOURCE: Institute of Physical Biochemistry, University of Munich, Munich, 80336, Germany
SOURCE: Biochemistry (1999), 38(2), 762-769
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

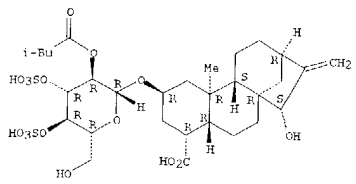
AB Nucleotide binding to the cytosolic binding site of the mitochondrial ADP/ATP carrier (AAC) was studied by 1H-NMR spectroscopy. Binding (as opposed to translocation) could be identified as a result of the rapid **ligand** on/off kinetics, using the cytosolic side specific inhibitor carboxyatractyloside (CAT) for the distinction from nonspecific interactions. The off rate constant of the nonhydrolyzable ATP analog AMP-PCP was more than 3 orders of magnitude larger than the transport rate. The nucleotides adopt an anti conformation in the carrier binding site as shown by measurements of the transferred nuclear Overhauser effect (TRNOE). A thermal transition around 14° that had been previously detected in transport studies [Klingenberg, M., Grebe, K., and Appel, M. (1982) Eur. J. Biochem. 126, 263-269] was reflected by the inhibitor sensitive line broadening, indicating that this transition also affects nucleotide binding. Nucleotide monophosphates were employed to study the relation between nucleotide structure and affinity, using selective excitation, sample spinning with digital suppression of spinning sidebands, and line shape simulation. The binding of purines depends on the distribution of the elec. potential and on the position of ring substituents, while pyrimidines are barely recognized at all by the AAC. It is also shown that the photocleavable "caged" derivs. are more tightly bound than the original nucleotides. A two step model of carrier catalysis will be discussed on the basis of these results.

IT **1398-13-6 33286-30-5**, Carboxyatractyloside
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(binding of nucleotides by mitochondrial ADP/ATP carrier as studied by 1H NMR spectroscopy)

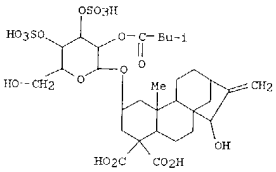
RN 1398-13-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L15 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 33286-30-5 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,15α)- (9CI) (CA INDEX NAME)



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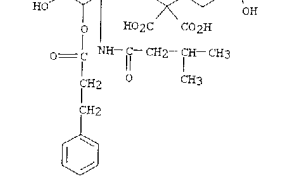
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1985:591696 CAPLUS
DOCUMENT NUMBER: 103:191696
TITLE: Wedeloside, a powerful inhibitor and **ligand** of the mitochondrial ADP/ATP carrier
AUTHOR(S): Klingenberg, Martin; Appel, Maria; Oelrichs, Peter B.
CORPORATE SOURCE: Inst. Phys. Biochem., Univ. Muenchen, Munich, 8000/2, Fed. Rep. Ger.
SOURCE: FEBS Letters (1985), 189(2), 245-9
CODEN: FEBLAL; ISSN: 0014-5793
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effect of wedeloside, an atractyloside analog from the Australian weed Wedelia asperrima, on the ADP/ATP carrier is investigated on 3 levels: ADP-stimulated respiration, ADP/ATP exchange, and binding competition with atractylate (ATR) and carboxyatractylate (CAT). The inhibition of respiration and of ADP/ATP exchange by wedeloside is nearly uncompetitive with ADP. The competitive binding with [3H]CAT and [3H]ATR reveals a high binding affinity of wedeloside, similar to that of CAT. Titration of ADP/ATP exchange and of the binding with wedeloside gives a titer of 0.35 μmol/g protein for rat liver protein and the titer of the binding gives 2.7 μmol/g protein for beef heart mitochondria. The titers are 1.8-fold higher than with CAT, suggesting that 2 mols. of wedeloside may bind to 1 ADP/ATP carrier dimer, in contrast to the half-site reactivity known for the binding of the other **ligands**.

IT **74686-30-9**
RL: BIOL (Biological study)
(adenine nucleotide-transporting protein of liver mitochondria binding and inhibition by)

RN 74686-30-9 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 2-[[2-deoxy-2-[(3-methyl-1-oxobutyl)amino]-3-O-(1-oxo-3-phenylpropyl)-β-D-glucopyranosyl]oxy]-13,15-dihydroxy-, (2β,15α)- (9CI) (CA INDEX NAME)



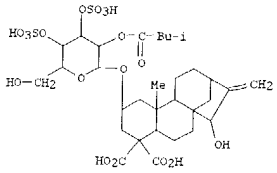
L15 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1985:433644 CAPLUS
DOCUMENT NUMBER: 103:33644
TITLE: Interaction of fluorescent 3'-[1,5-(dimethylamino)naphthoyl]adenine nucleotides with the solubilized ADP/ATP carrier
AUTHOR(S): Klingenberg, Martin; Mayer, Ingeborg; Appel, Maria
CORPORATE SOURCE: Inst. Phys. Biochem., Univ. Muenchen, Munich, 8000/2, Fed. Rep. Ger.
SOURCE: Biochemistry (1985), 24(14), 3650-9
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The binding of the 3'-[1,5-(dimethylamino)naphthoyl] (DAN) derivs. of AMP, ADP, and ATP to the solubilized ADP/ATP carrier was studied, evaluating primarily the fluorescence enhancement and 3H-labeled compound binding. DAN nucleotides also fluoresced when adsorbed to Triton X-100 micelles that are used for solubilization of the carrier. The partition of DAN-AMP between water and Triton X-100 micelles was measured, and was shifted toward a higher content in Triton micelles with increasing salt concentration In order to maintain a low level of fluorescence, the Triton content was decreased. The fraction of DAN nucleotide fluorescence due to carrier binding was determined by suppression with bongkrekate (BKA). In contrast to the membrane-bound carrier, the solubilized preparation showed an increase of total BKA-sensitive fluorescence by 30-60% upon addition of ATP or ADP. In the solubilized atractylate-protein complex, the ADP-stimulated fluorescence was 80%. The suppression of fluorescence by BKA was independent of the presence of ADP or ATP, whereas that by carboxyatractylate (CAT) depended on ADP or ATP. Quantitation with [3H]BKA and [3H]CAT of these **ligand** interactions with DAN-AMP fluorescence showed that DAN-AMP fluorescence reflects the m-state carrier population and its redistribution under the influence of ADP or ATP. Thus, besides the c/m distribution, the kinetics of the c-to-m transition in the solubilized carrier was also be determined The m share was increased to 80% when SO42-, inorg. phosphate, or pyrophosphate was present during solubilization. The rate of the ADP- or ATP-stimulated transition to the m state was markedly dependent on pH and on the presence of various anions, whereas the extent was little varied. The affinity decreased 4-fold going from DAN-AMP to DAN-ADP and to DAN-ATP (dissociation constant = 0.9, 1.6, and 3.2 μM, resp.). Comparison with phys. binding of [3H]DAN nucleotides showed that the fluorescence yield of bound DAN-AMP was .apprx.1.4-fold higher than that of bound DAN-ATP. DAN substitution caused >100-fold affinity increase for AMP and a 50-fold increase for ADP or ATP, probably because of interaction of the DAN group with a hydrophobic niche. A less specific, low-affinity displacement of DAN nucleotides by GDP, ADP, GTP, and ATP (Ki = 1-2 mM) probably reflects primarily the ionic interactions of the binding center.

IT **35988-42-2**
RL: BIOL (Biological study)
(adenine nucleotide (dimethylamino)naphthoyl derivative fluorescence quenching by, carrier protein binding in relation to)

RN 35988-42-2 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-α-D-glucopyranosyl]oxy]-, (2β,15α)- (9CI) (CA INDEX NAME)

L15 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L15 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

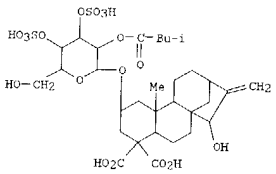
ACCESSION NUMBER: 1985:162405 CAPLUS
DOCUMENT NUMBER: 102:162405
TITLE: Substrate-induced modifications of the intrinsic fluorescence of the isolated adenine nucleotide carrier protein: demonstration of distinct conformational states
AUTHOR(S): Brandolin, Gerard; Dupont, Yves; Vignais, Pierre V.
CORPORATE SOURCE: Dep. Rech. Fondam., Cent. Etud. Nucl., Grenoble, 38041, Fr.
SOURCE: Biochemistry (1985), 24(8), 1991-7
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effects of ATP or ADP and the specific inhibitors carboxyatractyloside (CATR) and bongkrekic acid (BA) on the conformation of the isolated adenine nucleotide (AdN) carrier protein were studied by fluorescence spectroscopy. The addition of ATP to the AdN carrier resulted in a rapid fluorescence increase of the tryptophanyl residue(s) at 355 nm, which leveled off in <1 s at 22°. Among the natural nucleotides, only ATP and ADP were effective. At ≤10° the kinetics of the fluorescence increase induced by ATP were biphasic, consisting of a rapid phase (<1 s), followed by a slower phase that lasted for a few seconds and had virtually the same amplitude as the rapid one. Both phases were abolished when CATR was added prior to ATP and fully reversed when CATR was added after the fluorescence response to ATP had been elicited. The number of CATR-binding sites on the carrier protein was determined by CATR specific inhibition of the ATP-induced increase in intrinsic fluorescence. The calculated number of CATR sites was equal to that found by the CATR-induced release of the bound naphthoyl-ATP from the same preparation of AdN carrier, demonstrating the reliability of the intrinsic fluorescence assay. Addition of BA prior to or together with ATP nearly doubled the amplitude of the ATP-induced fluorescence signal. At ≤10° the fluorescence response to ATP in the presence of BA could also be decomposed into rapid and slow phases. The amplitude of the rapid phase was not modified in the presence of BA, but the amplitude of the slow phase was .apprx.3-fold higher than that of the rapid phase. The same results were obtained when ATP was replaced by ADP. In the absence of ATP, CATR itself modified the intrinsic fluorescence differently than did ATP, according to the excitation and emission spectra. These results are discussed on the basis of a minimal model where the AdN carrier is supposed to exist in 2 native conformations, the CATR and BA conformations that are trapped and stabilized by CATR and BA resp.; interconversion between the 2 conformations is triggered by ATP or ADP. On the basis of several observations that point to a tetrameric organization of the AdN carrier protein, it is suggested that the transition between the CATR and BA conformations is multiphasic and may proceed with sequential modification of each subunit of the tetramer.

IT **33286-30-5**
RL: PRP (Properties)
(conformation of adenine nucleotide-transporting protein response to, fluorescence in relation to)

RN 33286-30-5 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,15α)- (9CI) (CA INDEX NAME)

L15 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 K

L15 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

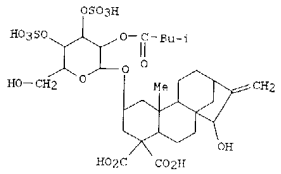
ACCESSION NUMBER: 1984:205184 CAPLUS
DOCUMENT NUMBER: 100:205184
TITLE: Interaction of fluorescent adenine nucleotide derivatives with the ADP/ATP carrier in mitochondria. 2. [5-(Dimethylamino)-1-naphthoyl]adenine nucleotides as probes for the transition between c and m states of the ADP/ATP carrier
AUTHOR(S): Klingenberg, Martin; Mayer, Ingeborg; Dahms, A. Stephen
CORPORATE SOURCE: Inst. Phys. Biochem., Univ. Muenchen, Munich, 8000/2, Fed. Rep. Ger.
SOURCE: Biochemistry (1984), 23(11), 2442-9
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The binding to the ADP/ATP carrier protein in mitochondrial membranes of the 3'-O-(dimethylamino)naphthoyl (DAN) derivs. of AMP, ADP, and ATP was quant. analyzed. The sideness of the fluorescent type binding to the matrix (m) side only was shown by comparing the mitochondrial membranes in various stages of integrity and surface orientation. In particles, displacement by bongkrekate (BKA) is direct, whereas in the case of carboxyatractylate (CAT); the requirement for ADP and ATP demonstrates the transition from the m to the c state. Quant. the phys. binding of [3H]DAN-AMP and fluorescence are well correlated, allowing for a little nonfluorescent binding to the c side. For DAN-AMP, KD is 1.6 μM, for DAN-ADP, KD is 0.8 μM, and in the Hill plot, a straight line with n = 1.25 is obtained. The maximum number of binding sites for [3H]DAN-AMP (1.5 μmol/g protein) is about equal to the sites found for [3H]BKA if the unspecific binding of both **ligands** is differentiated by blocking carrier sites with CAT. [3H]CAT binding is somewhat lower in accordance with the limited access of CAT to inverted vesicles. ADP is able to decrease fluorescence only by .apprx.35% at high concns. (10 mM), whereas GDP has virtually no effect. With ADP, DAN-AMP binding decreases by 30% of the total binding sensitive to BKA. Binding to ATPase is low because of the absence of Mg2+. The a priori identity of the 10-30% ADP-sensitive and therefore also exchange-active carrier sites with the 70-90% ADP-insensitive sites was established in comparative titrns. of the exchange, of binding, and of fluorescence with DAN-AMP, ADP, and BKA. DAN-AMP binding to whole mitochondria includes uptake which can be back-exchanged against external ADP. This implies binding of DAN nucleotides also to the c states of the carrier. In rat liver mitochondria, and energy-dependent regulation of DAN-ATP uptake, similar to that known for ATP, is observed These results indicate fluorescent, strong DAN nucleotide binding to the carrier in the m state and nonfluorescent, weak binding to the c state.

IT **35988-42-2**
RL: BIOL (Biological study)
(fluorescent adenine nucleotide derivative binding by carrier protein of mitochondria membrane response to, sidedness in)

RN 35988-42-2 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-α-D-glucopyranosyl]oxy]-, (2β,15α)- (9CI) (CA INDEX NAME)

L15 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L15 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

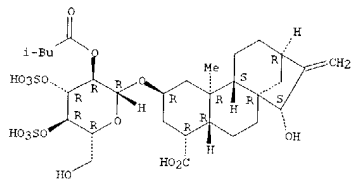
ACCESSION NUMBER: 1984:170191 CAPLUS
DOCUMENT NUMBER: 100:170191
TITLE: Probing the structure of the ADP/ATP carrier with pyridoxal phosphate
AUTHOR(S): Bogner, Werner; Aquila, Heinrich; Klingenberg, Martin
CORPORATE SOURCE: Inst. Phys. Biochem., Univ. Muenchen, Munich, 8000/2, Fed. Rep. Ger.
SOURCE: Developments in Bioenergetics and Biomembranes (1983), 6(Struct. Funct. Membr. Proteins), 145-56
CODEN: DBBIDG; ISSN: 0166-0861
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Pyridoxal phosphate (I) was used as a lysine-specific modifying reagent to probe the structure of the ADP/ATP carrier protein of beef heart mitochondria. By comparing the accessibilities of various lysine groups of the protein to I alone and in the presence of various **ligands** (atractylate, bongkrekate, and carboxyatractylate), a model for the conformational folding of the protein in the mitochondrial membrane was developed.

IT **1398-13-6 35988-42-2**
RL: BIOL (Biological study)
(lysine residue modification in adenine nucleotide-transporting protein of heart mitochondria by pyridoxal phosphate in presence of, protein conformational folding in relation to)

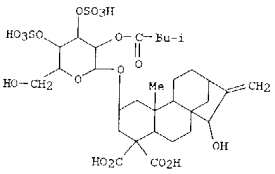
RN 1398-13-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 35988-42-2 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-α-D-glucopyranosyl]oxy]-, (2β,15α)- (9CI) (CA INDEX NAME)

L15 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L15 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

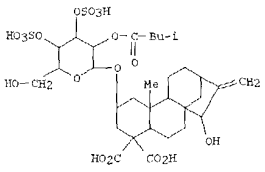
ACCESSION NUMBER: 1983:174956 CAPLUS
DOCUMENT NUMBER: 98:174956
TITLE: Use of 3'-O-naphthoyladenosine 5'-diphosphate to probe distinct conformational states of the membrane-bound ADP/ATP carrier
AUTHOR(S): Block, Marc R.; Lauquin, Guy J. M.; Vignais, Pierre V.
CORPORATE SOURCE: Dep. Rech. Fondam., Cent. Etud. Nucl., Grenoble, 38041, Fr.
SOURCE: Biochemistry (1983), 22(9), 2202-8
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The fluorescent ADP analog, 3'-O-naphthoyl-ADP (I), which binds to the mitochondrial ADP/ATP carrier (adenine nucleotide translocase) (II) but is not transported, was used to probe the interactions with II of 2 specific inhibitors, carboxyatractyloside (III) and bongkrekic acid (IV), both in heart mitochondria and in inside out submitochondrial particles obtained by sonication of mitochondria (sonic particles). III and IV are mutually exclusive for binding; moreover, in mitochondria, III attacks II from the outside, and IV from the inside, whereas in sonic particles the reverse is true. The mitochondria and sonic particles were loaded with I, and the amount of II-bound I released upon addition of III and IV was monitored fluorometrically. The kinetics of I release could be easily resolved by lowering the temperature In mitochondria, the release was clearly biphasic at 10°; the 1st phase induced by III corresponded to the release of 40-70% of the II-bound I and lasted for <0.5 s; it ended abruptly and was followed by a very slow release of the rest of II-bound I, which required >20 min for completion. Addition of IV at the onset of the slow phase dramatically accelerated the release of I; acceleration also occurred upon addition of micromolar concns. of ADP or any transportable nucleotide. Reversing the sequence of addns., i.e., starting by the addition of IV, led to similar results, namely, a 2-step release of the bound I, consisting of a rapid phase of partial release of bound I followed by a slow one that was accelerated by III or ADP. In the case of sonic particles loaded with I, IV was able to induce the extensive release of II-bound I at 10°, either in the absence or presence of ADP. On the other hand, III was inefficient in releasing bound I at 10°, unless ADP or another transportable nucleotide was added. These data provide the 1st direct exptl. evidence in favor of a II model in which the III or IV conformations exist prior to the addition of III or IV. Any given II unit in the mitochondrial membrane is suggested to exist either in the III conformation or in the IV conformation. Bound I would be released upon binding either of III to those II units in the III conformation or of IV to those in the IV conformation. In heart mitochondria, 40-70% of the II units would be in the III conformation, depending on the nature of the preparation, the remainder being in the IV conformation. In sonic particles, however, most of the II units would be in the IV conformation. The transition between the III and IV conformations is very slow at 10°; it is increased by raising the temperature or by adding micromolar concns. of ADP or any transportable nucleotide, suggesting that it is an intrinsic event in ADP/ATP transport.

IT **33286-30-5**
RL: BIOL (Biological study)
(adenine nucleotide carrier binding of, conformational states in relation to)

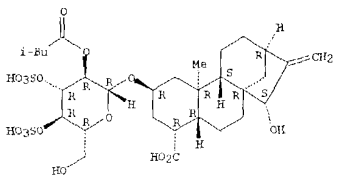
RN 33286-30-5 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-

L15 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,15α)- (9CI) (CA INDEX NAME)



●2 K

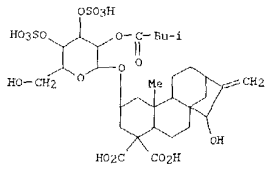
L15 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



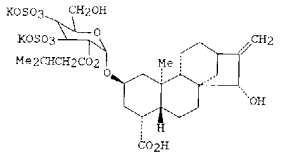
L15 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1983:13577 CAPLUS
DOCUMENT NUMBER: 98:13577
TITLE: Studies on the interaction of palmitoyl-coenzyme A with the adenine nucleotide translocase
AUTHOR(S): Woldegiorgis, Gebretateos; Yousufzai, Sardar Y. K.; Shrago, Earl
CORPORATE SOURCE: Dep. Med., Univ. Wisconsin, Madison, WI, 53706, USA
SOURCE: Journal of Biological Chemistry (1982), 257(24), 14783-7
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Palmitoyl-CoA which can inhibit adenine nucleotide transport from both the cytosolic and matrix sides of the inner mitochondrial membrane removed bound [14C]ADP from the cytosolic side of intact mitochondria but not from the matrix side of submitochondrial particles with inverted sidedness. The ADP-stimulated binding of [14C]-N-ethylmaleimide to mitochondria, which can be prevented by atractylate, was also inhibited by palmitoyl-CoA with isolated mitochondria but not submitochondrial particles. Two analogs of palmitoyl-CoA were synthesized and tested for their ability to inhibit adenine nucleotide translocation in mitochondria and submitochondrial particles. 1-N6-Ethenopalmitoyl-CoA closely resembled palmitoyl-CoA in its action, whereas dephosphopalmitoyl-CoA was completely ineffective at the same concentration. Mitochondria and submitochondrial particles were incubated with [14C]palmitoyl-CoA and the [14C]palmitoyl-CoA-protein complexes were purified by extraction with Triton X-100 and hydroxyapatite chromatog. The elution profiles of radioactivity and protein resembled those obtained with radioactive carboxyatractylate and bongkrekic acid and represent the purified ADP/ATP carrier. The palmitoyl-CoA **ligand** conferred stability on the protein, particularly against trypsin digestion, when the palmitoyl-CoA protein complex was purified from isolated mitochondria. However, when the protein complex was purified from submitochondrial particles, palmitoyl-CoA was less able to prevent trypsin digestion. Again, these characteristics are similar to those of the resp. carboxyatractylate and bongkrekic acid protein complexes. These results indicate a site-specific interaction of palmitoyl-CoA with the ADP/ATP carrier and support the concept that long-chain fatty acyl-CoA esters are natural **ligands** for the carrier.
IT **1398-13-6**
RL: BIOL (Biological study)
(adenine nucleotide translocase interaction with, palmitoyl-CoA in relation to)
RN 1398-13-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L15 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1982:99710 CAPLUS
DOCUMENT NUMBER: 96:99710
TITLE: Incorporation of N-ethylmaleimide into the membrane-bound ADP/ATP translocator. Isolation of the protein labeled with N-[3H]ethylmaleimide
AUTHOR(S): Aquila, Heinrich; Eiermann, Wolfgang; Klingenberg, Martin
CORPORATE SOURCE: Inst. Phys. Biochem., Univ. Muenchen, Munich, D-8000/2, Fed. Rep. Ger.
SOURCE: European Journal of Biochemistry (1982), 122(1), 133-9
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The incorporation of N-ethylmaleimide into the 30,000-mol. weight (Mr) component of beef heart mitochondria was studied as a function of various **ligands** to the ADP/ATP carrier and the isolation of the N-ethylmaleimide-labeled protein is reported. The incorporation of N-ethylmaleimide into the 30,000-Mr component is specifically stimulated by ADP and ATP. Thus, by differential incorporation of N-ethylmaleimide, the 30,000-Mr component is preferentially labeled. Addition of carboxyatractylate inhibits, whereas bongkrekate tolerates, the incorporation of N-ethylmaleimide. After solubilization by Triton, the purification of N-ethylmaleimide-labeled protein is facilitated in the presence of bongkrekate but not of carboxyatractylate, in agreement with the postulated existence of only a bongkrekate-N-ethylmaleimide-protein complex. The labeled protein was purified to homogeneity on hydroxylapatite in Triton and subsequently, after denaturation in SDS, on Sepharose 6B. The identity of the isolated labeled protein with the formerly isolated bongkrekate-protein or carboxyatractylate-protein complexes is confirmed by the isoelec. point and amino acid composition. Two moles of N-ethylmaleimide must be incorporated into the 30,000-Mr component in order to inhibit fully the binding of 1 mol carboxyatractylate. This corresponds to 1 SH group/unit.
IT **35988-42-2**
RL: BIOL (Biological study)
(adenine nucleotide translocase labeling by ethylmaleimide response to)
RN 35988-42-2 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[(2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-α-D-glucopyranosyl]oxy]-, (2β,15α)- (9CI) (CA INDEX NAME)



L15 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1981:203144 CAPLUS
DOCUMENT NUMBER: 94:203144
TITLE: Chemical modifications of atractyloside and bongkrekic acid binding sites of the mitochondrial adenine nucleotide carrier. Are there distinct binding sites?
AUTHOR(S): Block, Marc R.; Lauquin, J. M.; Vignais, Pierre V.
CORPORATE SOURCE: Dep. Rech. Fondam., CEN Grenoble, Grenoble, 38041, Fr.
SOURCE: Biochemistry (1981), 20(9), 2692-9
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

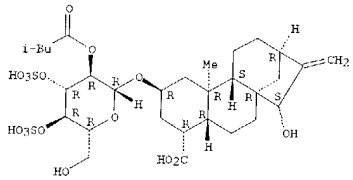


I

AB The nature of the binding sites for 2 specific inhibitory **ligands** of the ADP/ATP carrier in beef heart mitochondria was investigated by means of chemical modifications with 2-hydroxy-5-nitrobenzyl bromide (HNB), a rather selective reagent for tryptophanyl residues, and 2,3-butanedione and phenylglyoxal, 2 reagents which modify arginyl residues. Atractyloside (I) [**17754-44-8**] binding, but not bongkrekic acid [11076-19-0] binding, was rapidly inactivated by HNB. I binding was also rapidly inactivated by butanedione and phenylglyoxal whereas bongkrekic acid binding was only slowly inactivated by these reagents. In all cases inactivation decreased the number of high-affinity binding sites without modification of the Kd value of the remaining sites; furthermore, specific protection of I or bongkrekic acid binding was afforded by preincubation with the homologous **ligand**. Inhibition of I binding by HNB was accompanied by the binding of HNB to the ADP/ATP carrier protein. Protection against HNB inhibition by preincubation of mitochondria with I was correlated with a decrease in the amount of bound HNB. Both I and bongkrekic acid bindings were inhibited by phenylglyoxal and butanedione, but the binding of I was inactivated ≥3 times faster than that of bongkrekic acid by these reagents. The reaction order with respect to phenylglyoxal concentration was 1 for inactivation of I binding and 2 for inactivation of the bongkrekic acid binding. Inactivation of I and bongkrekic acid binding by phenylglyoxal was studied as a function of the specific binding of [14C]phenylglyoxal, sensitive to I and bongkrekic acid, resp. Complete inactivation of I binding required the incorporation of 1 mol of [14C]phenylglyoxal per mol of carrier dimer (Mr 60,000), indicating a mechanism of half-site reactivity for the I site of the ADP/ATP carrier. Full inactivation of bongkrekic acid binding required at

L15 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
least twice as much phenylglyoxal. The ADP/ATP carrier protein is apparently an asym. protein spanning the inner mitochondrial membrane, its asymmetry being reflected by distinct preexisting binding sites for I and bongkrekic acid.
IT **17754-44-8**
RL: PRP (Properties)
(adenine nucleotide carrier protein binding sites for, in mitochondria)
RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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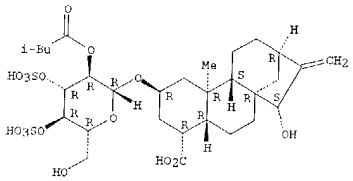
L15 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1979:147158 CAPLUS
DOCUMENT NUMBER: 90:147158
TITLE: Phosphate dependence and atractyloside inhibition of mitochondrial oxidative phosphorylation. The ADP-ATP carrier is rate-limiting
AUTHOR(S): Lemasters, John J.; Sowers, Arthur E.
CORPORATE SOURCE: Dep. Anat., Univ. North Carolina, Chapel Hill, NC, USA
SOURCE: Journal of Biological Chemistry (1979), 254(4), 1248-51
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
AB ATP production and O consumption by rat liver mitochondria were measured as a function of atractyloside and phosphate (Pi) concentration. The "on" kinetics of atractyloside inhibition of ATP production are very rapid, and the onset of inhibitory effect is complete within 1 s even at concns. which produce partial inhibition. A **ligand** conservation plot relating atractyloside concentration and fractional inhibition of ATP production is linear and indicates that inhibition is proportional to the fraction of ADP-ATP carrier sites bound with atractyloside. Ests. of E, the number of atractyloside sensitive sites, and Ki, the atractyloside inhibition constant, are 3.8 + 10-7 mol/g of protein and 2.2 + 10-8M, resp. Mitochondrial respiration during active oxidative phosphorylation is proportional to log [Pi]. Plots of atractyloside concentration vs. respiratory rate at different Pi concns. are similar in shape. There is no increase in sigmoidicity with decreasing Pi that would suggest that the ADP-ATP carrier is losing any rate-limiting character as Pi decreases and the rate of the reaction falls. Hexokinase at concns. below .apprx.400 units/g of mitochondrial protein limits the rate of mitochondrial respiration in the presence of glucose and ATP. Atractyloside inhibition curves become increasingly sigmoidal as hexokinase is decreased below 400 units/g of protein. Thus, when the ADP-ATP carrier is not rate-limiting, significant amts. of atractyloside can bind without producing a corresponding decrease in ATP production. In rat liver mitochondria, adenine nucleotide translocation is rate-limiting in the overall reaction of oxidative phosphorylation and is responsible for the phenomenon of respiratory control.
IT **17754-44-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidative phosphorylation response to, rate-limiting adenine nucleotide transport in relation to)
RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

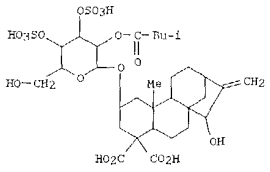
Absolute stereochemistry.

L15 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



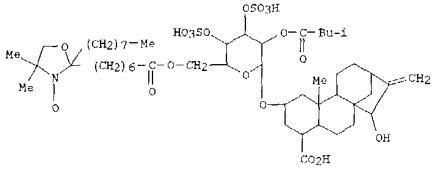
●2 K

L15 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:102253 CAPLUS
DOCUMENT NUMBER: 88:102253
TITLE: The adenine nucleotide translocator in fetal, suckling and adult rat liver mitochondria
AUTHOR(S): Pollak, J. K.; Sutton, Rosemary; Klingenberg, Martin
CORPORATE SOURCE: Dep. Histol. Embryol., Univ. Sydney, Sydney, Australia
SOURCE: Biochemical and Biophysical Research Communications (1978), 80(1), 193-8
CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The adenine nucleotide content of rat liver mitochondria increased significantly after birth. On the other hand, the **ligand**-binding properties of the adenine nucleotide translocator were essentially the same in fetal, suckling, and adult rat liver mitochondria. These results are compatible with the proposal that the accumulation of adenine nucleotides which occurs during mitochondrial biogenesis and maturation is effected by a pathway different from the adenine nucleotide translocator.
IT **35988-42-2**
RL: BIOL (Biological study)
(adenine nucleotide translocator binding of, development in relation to)
RN 35988-42-2 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-α-D-glucopyranosyl]oxy]-, (2β,15α)- (9CI) (CA INDEX NAME)



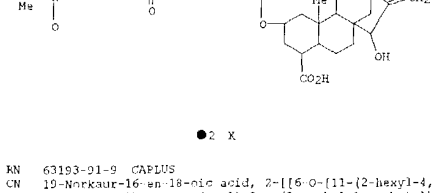
L15 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:166506 CAPLUS
DOCUMENT NUMBER: 86:166506
TITLE: Spin-labeled acyl atractyloside as a probe of the mitochondrial adenosine diphosphate carrier. Asymmetry of the carrier and direct lipid environment
AUTHOR(S): Lauquin, Guy J. M.; Devaux, Philippe F.; Bienvenue, Alain; Villiers, Christian; Vignais, Pierre V.
CORPORATE SOURCE: Dep. Rech. Fondam., CEN, Grenoble, Fr.
SOURCE: Biochemistry (1977), 16(6), 1202-8
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A number of spin-labeled acyl deriva. of atractyloside, (m,n)acyl-ATR (general formula: CH3(CH2)mCX(CH2)nCOO-ATR, where X is an oxazolidine ring containing a nitroxide), were synthesized and used to probe the ADP carrier in heart mitochondria. They inhibit ADP transport with the same efficiency as unlabeled acyl-ATRs. The inhibition is a mixed competitive and noncompetitive inhibition. The long chain acyl-ATRs ((10,3)-, (7,6)-, (7,8)-, and (5,10)acyl-ATRs) and also the short chain (0,2)acyl-ATR, when added at low concns. to heart mitochondria, give rise to more immobilized ESR spectra than when added to liposomes. On addition of atractyloside or of other specific **ligands**, spin-labeled long-chain acyl-ATRs bound to the ADP carrier are displaced from their binding site toward the lipid phase of the mitochondrial membrane and the short chain (0,2)acyl-ATR is released into the aqueous phase. Spin-labeled long-chain acyl-ATRs do not show any evidence of binding to a protein when incubated with inside out submitochondrial particles, in spite of the fact that these particles are able to transport ADP. These results are discussed with respect to the size and the asymmetry of the ADP carrier in the mitochondrial membrane and the mechanism of ADP transport.
IT **63193-89-5 63193-90-8 63193-91-9**
**63193-92-0 63193-93-1 63196-04-3**
RL: BIOL (Biological study)
(as mitochondrial membrane probe)
RN 63193-89-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[7-(4,4-dimethyl-2-octyl-3-oxy-2-oxazolidinyl)-1-oxoheptyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L15 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 K

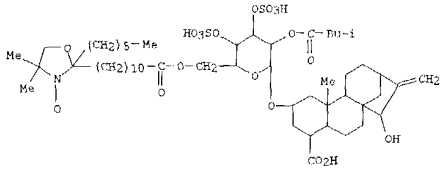
RN 63193-90-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-[9-(4,4-dimethyl-2-octyl-3-oxy-2-oxazolidinyl)-1-oxononyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)



●2 K

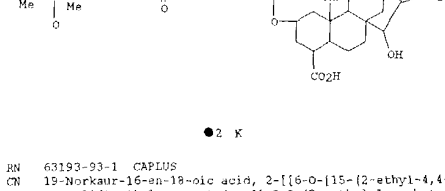
RN 63193-91-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[11-(2-hexyl-4,4-dimethyl-3-oxy-2-oxazolidinyl)-1-oxoundecyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L15 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 K

RN 63193-92-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-[1-oxo-2-(2,4,4-trimethyl-3-oxy-2-oxazolidinyl)propyl]-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)



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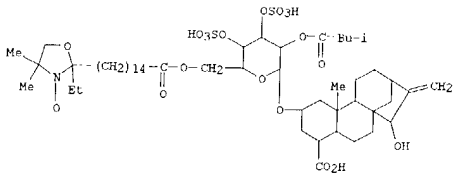
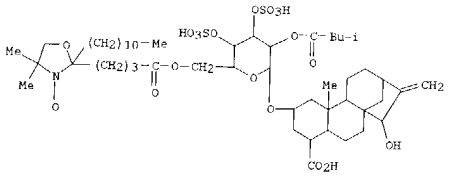
RN 63193-93-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[15-(2-ethyl-4,4-dimethyl-3-oxy-2-oxazolidinyl)-1-oxopentadecyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L15 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 K

RN 63196-04-3 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-(4,4-dimethyl-3-oxy-2-undecyl-2-oxazolidinyl)-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)



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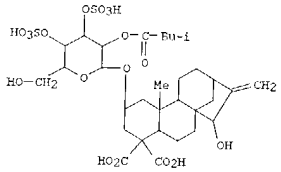
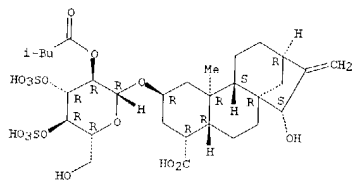
L15 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1976:473737 CAPLUS
DOCUMENT NUMBER: 85:73737
TITLE: Characterization of the isolated ADP,ATP carrier
AUTHOR(S): Klingenberg, M.; Aquila, H.; Riccio, P.; Buchanan, B. B.; Eiermann, W.; Hackenberg, H.
CORPORATE SOURCE: Inst. Physiol. Chem. Phys. Biochem., Univ. Muenchen, Munich, Fed. Rep. Ger.
SOURCE: Electron Transfer Chains Oxid. Phosphorylation, Proc. Int. Symp. (1975), 431-8. Editor(s): Quagliariello, E.; Papa, S.; Palmieri, F. North-Holland: Amsterdam, Neth.
CODEN: 33KUA4
DOCUMENT TYPE: Conference
LANGUAGE: English
AB A pure and homogeneous carboxyatractylate (I)-binding protein was isolated from beef heart mitochondria. The protein has a monomer mol. weight of 29,000 on Na dodecyl sulfate-polyacrylamide gel electrophoresis and appears to bind a single I mol. in a dimer form of mol. weight 67,000. The effectivity of I displacement by nucleotide **ligands** parallels the biol. transport carrier specificity in situ; thus, the I-binding protein is identical to the adenine nucleotide carrier. The isolated carrier is subject to different conformational and functional states. Removal of I by ADP, which forms a looser short-lived complex, leads to proteolytic degradation of an inactive (nonbinding) denatured form. The release of I by bongkrekate plus ADP is inhibited by antibodies to the I-binding protein, possibly as a result of the inhibition of a conformation change. Bonkrekate protects the native m-state conformation of the carrier. The mechanism of transport catalysis is briefly discussed.
IT **35988-42-2**
RL: BIOL (Biological study)
(protein binding, of mitochondria)
RN 35988-42-2 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-α-D-glucopyranosyl]oxy]-, (2β,15α)- (9CI) (CA INDEX NAME)



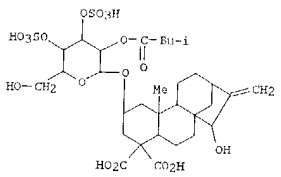
L15 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:151000 CAPLUS
DOCUMENT NUMBER: 82:151000
TITLE: Binding of atractylate and carboxy-atractylate to mitochondria
AUTHOR(S): Klingenberg, Martin; Grebe, Karin; Scherer, Burkhard
CORPORATE SOURCE: Inst. Physiol. Chem. Phys. Biochem., Univ. Muenchen, Munich, Fed. Rep. Ger.
SOURCE: European Journal of Biochemistry (1975), 52(2), 351-63
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 35S-labeled atractylate and carboxyatractylate were produced biosynthetically and used for studying the binding of these specific **ligands** to the ADP-ATP carrier in beef heart mitochondria. Inhibition of translocation activity was parallel to the increase of binding by atractylate-35S. No addnl. binding was observed after full inhibition of translocation was reached, indicating that atractylate binds exclusively to the carrier. The maximum number of binding sites of both atractylates was .apprx.1.6 μmole/g protein in beef heart mitochondria and decreased on treatment of the membrane by phosphate (Pi), freezing, ageing, etc. The dissociation consts. of the binding were approx. for atractylate Kd = 5 + 10-8M and for carboxyatractylate Kd = 10-8M. The mass action plots of the concentration dependence for the binding were nonlinear-convex, in particular with carboxyatractylate and more linear with atractylate. Nonlinearity appeared to be caused by some retardation of equilibration in the case of very high affinity binding. The binding of atractylate and carboxyatractylate was relatively fast in intact mitochondria and slower in aged membranes. There was a slower and a faster binding portion. The atractylates removed ADP in a nearly 1:1 stoichiometry from untreated mitochondria. In aged and Pi-treated membranes the ratio ΔADP/Δatractylate approached 0. Obviously, binding of carrier sites to ADP is more sensitive to alterations then that of the atractylates. The assumption is maintained that the binding site for atractylate is identical with that for ADP and ATP. Bongkrekate prevented binding of both atractylates. However, when added after, it only removed atractylate but not the carboxy compound because of its different tight binding. The removal of atractylate depended on the synergistic effect of bongkrekate with ADP. The binding studies with atractylate and in particular the interaction with bongkrekate support the reorienting carrier model in which atractylate as an impermeable **ligand** fixes the binding site of the carrier outside whereas with bongkrekate the carrier site is turned to the inside.
IT **1398-13-6 35988-42-2**
RL: BIOL (Biological study)
(mitochondria binding of, ADP transport in relation to)
RN 1398-13-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L15 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



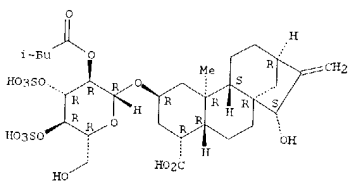
RN 35988-42-2 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-α-D-glucopyranosyl]oxy]-, (2β,15α)- (9CI) (CA INDEX NAME)



L15 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1974:141433 CAPLUS
DOCUMENT NUMBER: 80:141433
TITLE: Mechanism of bongkrekate effect on the mitochondrial adenine nucleotide carrier studied by the binding of ADP
AUTHOR(S): Klingenberg, Martin; Buchholz, Marlies
CORPORATE SOURCE: Inst. Physiol. Chem. Phys. Biochem., Univ. Muenchen, Munich, Fed. Rep. Ger.
SOURCE: European Journal of Biochemistry (1973), 38(2), 346-58
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Effects of bongkrekate (I) on binding of ADP [58-64-0] to the inner mitochondrial membrane demonstrated the reorientation of a mobile carrier across the membrane. The dependence of the I-induced increase of ADP binding was nonlinear with respect to the I concentration The binding of I was dependent on ADP indicating a reciprocal enhancement effect between ADP and I binding. The counteraction of I and atractylate [**17754-44-8**] on ADP binding depended on the cooperation between ADP and I. The I-induced ADP binding was irreversible. Thus, there seems to be a reorientation mechanism of the I effect by which the ADP carrier complex is translocated inside and all carriers become trapped inside by I as the immobile carrier-I complex. The reciprocal enhancement of I and ADP binding is explained by the fact, that ADP is required to move the carrier inside where I can bind to the carrier. The irreversibility of the I effect results from the shift of the carrier inside and the resulting removal of the carrier out of the equilibrium with external **ligands** such as atractylate or ADP.
IT **17754-44-8**
RL: PRP (Properties)
(ADP binding response to, in heart mitochondria, bongkrekate in relation to)
RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L15 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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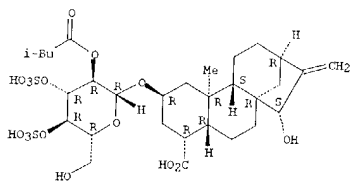
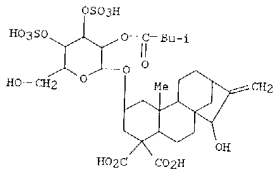
L15 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1974:56625 CAPLUS
DOCUMENT NUMBER: 80:56625
TITLE: Demonstration of the relation between the adenine nucleotide carrier and the structural changes of mitochondria as induced by adenosine 5'-diphosphate
AUTHOR(S): Scherer, Burkhard; Klingenberg, Martin
CORPORATE SOURCE: Inst. Phys. Biochem., Univ. Munich, Munich, Fed. Rep. Ger.
SOURCE: Biochemistry (1974), 13(1), 161-70
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The specific interaction of various **ligands** with the mitochondrial ADP carrier was explored on the basis of structural changes of mitochondria (as measured by absorbance changes) and the binding of ADP-14C. A detailed insight into the function of a membrane carrier was obtained which strongly supported the mobile carrier model on a mol. basis. The linkage of absorbance changes at 546 nm to the binding of ADP at the carrier was demonstrated by quant. agreement between absorbance change and binding extent. The absorbance increase (i.e., contraction of mitochondria matrix) had a low Km for ADP (4 μM), similar to that for ADP binding to the carrier. The contraction was also highly specific for ADP and ATP. From the absorbance decrease (expansion) induced by atractylate an apparent Kd = 3 + 10-8M was obtained, in agreement with atractylate-35S-binding studies. In contrast to atractylate, bongkrekate further increased the absorbance, in agreement with binding studies. In general, depending on time and on bongkrekate concentration, the increases of absorbance and of binding occurred in parallel. The rate of the bongkrekate-induced absorbance increase was relatively slow and increased strongly with H+ concentration, indicating a requirement for diffusion of undissocd. bongkrekate through the membrane. The rate of the bongkrekate effect had a high temperature dependence (EA = 23 kcal). The bongkrekate-induced absorbance increase was competitively inhibited by atractylate and completely inhibited by carboxyatractylate. The results are best explained by postulating that absorbance changes reflect carrier localization on the inner surface or the outer surface. The expanded state is associated with the accumulation of carrier on the outer surface and the contracted state with its accumulation on the inner surface. Atractylate as an impermeable **ligand** traps the carrier on the outside whereas bongkrekate as a permeable **ligand** fixes and traps the carrier on the inside. In both cases the carrier is immobilized. On binding ADP, the carrier becomes mobile and distributes both on the inside and outside according to the ADP concentration gradient.
IT **1398-13-6 35988-42-2**
RL: BIOL (Biological study)
(adenine nucleotide carrier binding of, mitochondria structure in relation to)
RN 1398-13-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L15 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 35988-42-2 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-α-D-glucopyranosyl]oxy]-, (2β,15α)- (9CI) (CA INDEX NAME)



L15 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

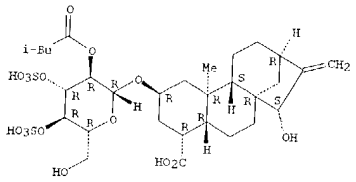
ACCESSION NUMBER: 1973:414784 CAPLUS
DOCUMENT NUMBER: 79:14784
TITLE: New atractyloside type compound as a high affinity **ligand** to the adenine nucleotide carrier
AUTHOR(S): Scherer, B.; Grebe, K.; Riccio, P.; Klingenberg, M.
CORPORATE SOURCE: Inst. Physiol. Chem. Phys. Biochem., Univ. Muenchen, Munich, Fed. Rep. Ger.
SOURCE: FEBS Letters (1973), 31(1), 15-19
CODEN: FEBLAL; ISSN: 0014-5793
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The binding of carboxyatractyloside-35S (I), atractyloside-35S (II), and epiatractyloside-35S (III) to beef heart mitochondria was compared. When I, II, and III were added simultaneously, there was no difference in competition. If III was added first, the subsequent addition of I and II did not remove III. Reversing the sequence resulted in III being prevented from binding completely by I and up to 85% by II. The high affinity for III was close to that for I. The explanation may lie in their common equatorial carboxyl group.

IT **17754-44-8 35988-42-2 42437-59-2**
RL: BIOL (Biological study)
(mitochondria membrane binding by, adenine nucleotides in)

RN 17754-44-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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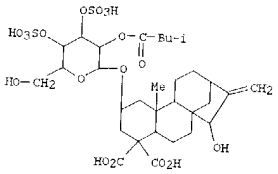
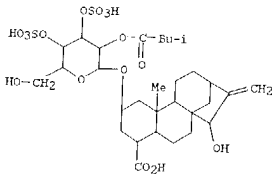
RN 35988-42-2 CAPLUS
CN Kaur-16-ene-18,19 dioic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-α-D-glucopyranosyl]oxy]-, (2β,15α)- (9CI) (CA INDEX NAME)

L15 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 42437-59-2 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-α-D-glucopyranosyl]oxy]-, (2β,4β,15α)- (9CI) (CA INDEX NAME)



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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 MAR 2004 HIGHEST RN 668418-93-7
DICTIONARY FILE UPDATES: 28 MAR 2004 HIGHEST RN 668418-93-7

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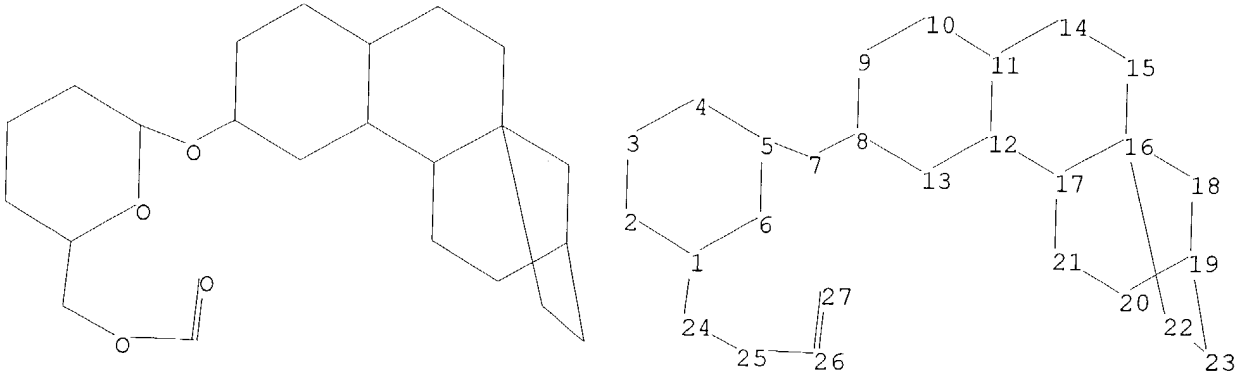


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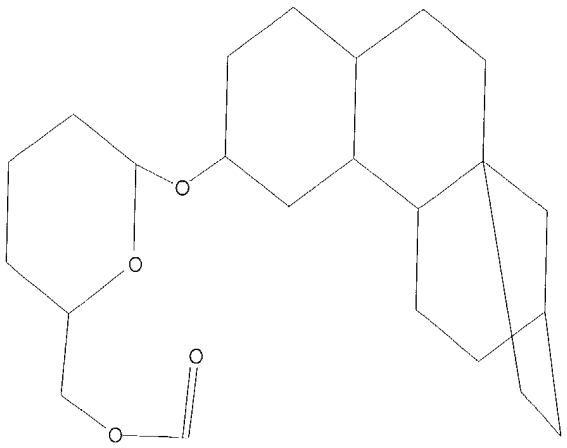


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FILE COVERS 1907 - 29 Mar 2004  VOL 140 ISS 14
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  This file contains CAS Registry Numbers for easy and accurate
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L20 ANSWER 1 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:465960 CAPLUS
DOCUMENT NUMBER: 137:47439
TITLE: Preparation of amino acid derivatives for altering mitochondrial function and cellular responses
INVENTOR(S): Pei, Yazhong; Moos, Walter H.; Ghosh, Soumitra S.
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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| WO 2002048092 | A2 | 20020620 | WO 2001-US48068 | 20011214 |
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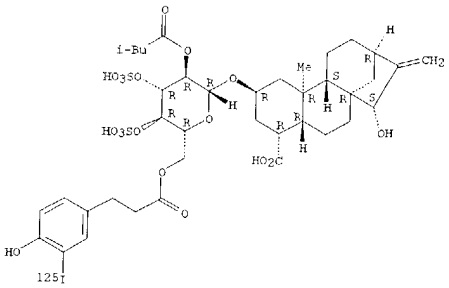
PRIORITY APPLN. INFO.: US 2000-255803P P 20001215
WO 2001-US48068 W 20011214
OTHER SOURCE(S): MARPAT 137:47439
AB Compds. R1COCHR2N(CH2CO2H)CO-A-C6H4NHCOR3 [A is a direct bond, (un)substituted alkyldiyl, -O-(alkyldiyl)-, -(alkyldiyl)-O-, -N(R')-(alkyldiyl)- (R' = H or alkyl), -(alkyldiyl)-N(R')-, heterocyclediyl, or heterocyclealkyldiyl; R1 = OH, alkoxy, aryloxy, arylalkyloxy, amino, or mono- or dialkylamino; R2 = H, (un)substituted alkyl, aryl, arylalkyl, heterocyclyl, or heterocyclylalkyl; R3 = (un)substituted alkyl, aryl, arylalkyl, heterocyclyl, or heterocyclylalkyl] were prepared for treating diseases by altering mitochondrial function that affects cellular processes. Thus, (HO2CCH2)2NCOC6H4NHAc-o was prepared by substitution reaction of glycine tert-Bu ester acetate with bromoacetate resin, reaction with 2-nitrobenzoic acid, nitro group reduction, acetylation with Ac2O, and resin cleavage using TFA. Biol. activities of compds. of the invention were examined in neuronal viability, displacement of an adenine nucleotide translocase ligand from isolated mitochondria, and chondrocyte cytodeprotection assays.
IT **437992-74-0**
RL: BSU (Biological study, unclassified); BIOL (Biological study) (radioligand; measurement of binding efficacy of amino acid derivs. in relation to mitochondrial function and cellular responses)
RN 437992-74-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-[4-hydroxy-3-(iodo-125I)phenyl]-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX

L20 ANSWER 1 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
NAME)

Absolute stereochemistry.



L20 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:833514 CAPLUS
DOCUMENT NUMBER: 136:1609
TITLE: Production of adenine nucleotide translocator (ANT) with recombinant cells, ANT ligands and screening assays therefor
INVENTOR(S): Anderson, Christen M.; Davis, Robert E.; Clevenger, William; Wiley, Sandra Eileen; Miller, Scott W.; Szabo, Tomas R.; Ghosh, Soumitra S.; Moos, Walter H.; Pei, Yazhong; Carroll, Amy K.
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 147 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001085944 | A2 | 20011115 | WO 2001-US15416 | 20010511 |
| WO 2001085944 | A3 | 20020829 | | |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

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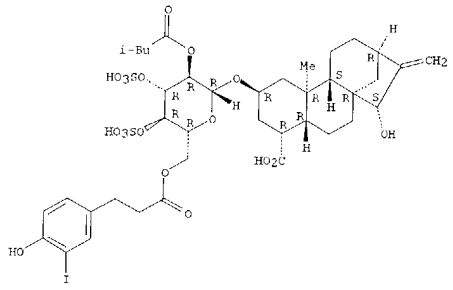
|---|---|---|---|---|
| EP 1283884 | A2 | 20030219 | EP 2001-935420 | 20010511 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| JP 2003532420 | T2 | 20031105 | JP 2001-582533 | 20010511 |

PRIORITY APPLN. INFO.: US 2000-569327 A 20000511
WO 2001-US15416 W 20010511
OTHER SOURCE(S): MARPAT 136:1609
AB Compns. and methods are provided for producing adenine nucleotide translocator (ANT) polypeptides and fusion proteins, including the production and use of recombinant expression constructs having a regulated promoter. ANT ligands and compns. and methods for identifying ANT ligands, agents that bind ANT and agents that interact with ANT are also disclosed. Thus, ANT cDNAs were expressed in Sf9 and E.coli. Fluorescent and radiolabeled derivs. of atractyloside were prepared. Binding of these derivs. to ANT was examined
IT **267886-33-9P 267886-35-1P 267886-37-3P**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(production of adenine nucleotide translocator (ANT) with recombinant cells, ANT ligands and screening assays therefor)
RN 267886-33-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxy-3-iodophenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

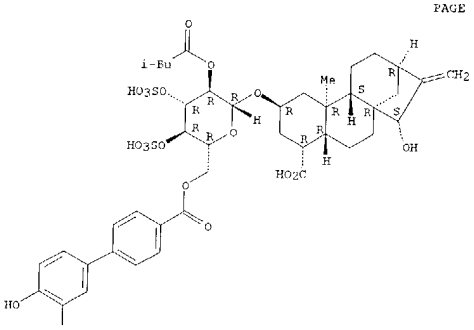
L20 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-35-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[(4'-hydroxy-3'-iodo[1,1'-biphenyl]-4-yl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





L20 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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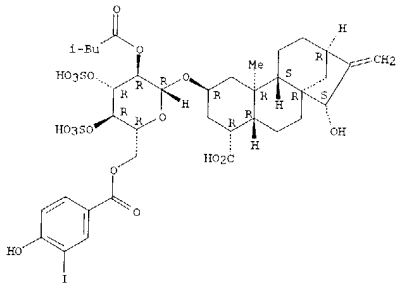
RN 267886-37-3 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-(4-hydroxy-3-iodobenzoyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

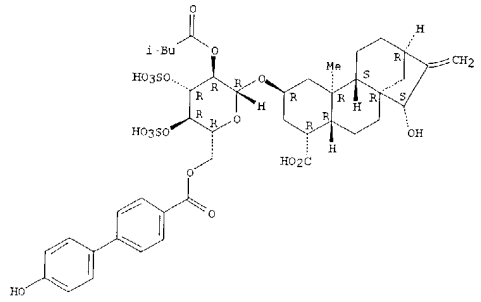
Absolute stereochemistry.



IT **267886-34-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(production of adenine nucleotide translocator (ANT) with recombinant cells, ANT ligands and screening assays therefor)
RN 267886-34-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[(4'-hydroxy[1,1'-biphenyl]-4-yl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L20 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT **267886-39-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(production of adenine nucleotide translocator (ANT) with recombinant cells, ANT ligands and screening assays therefor)
RN 267886-39-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-[[2-(4-hydroxyphenyl)ethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L20 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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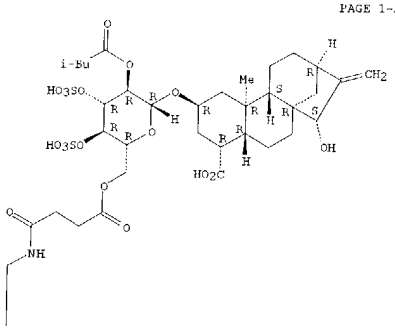
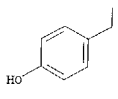


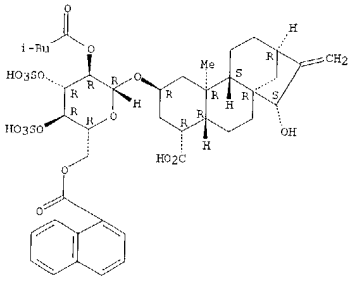
PAGE 2-A



IT **84882-67-7P 267886-17-9P 267886-18-0P**
**267886-21-5P 267886-32-8P 267886-36-2P**
**267886-38-4P 267886-40-8P 267886-41-9P**
**267886-42-0P 267886-43-1P 267886-44-2P**
**267886-45-3P 267886-46-4P 267886-47-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(production of adenine nucleotide translocator (ANT) with recombinant cells, ANT ligands and screening assays therefor)
RN 84882-67-7 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-(1-naphthalenylcarbonyl)-2,3-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

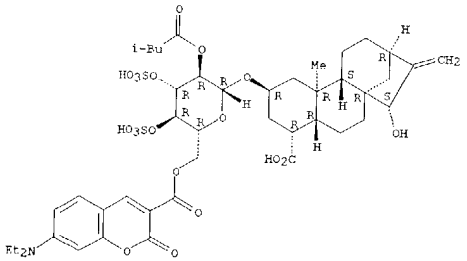
Absolute stereochemistry.

L20 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-17-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[[7-(diethylamino)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

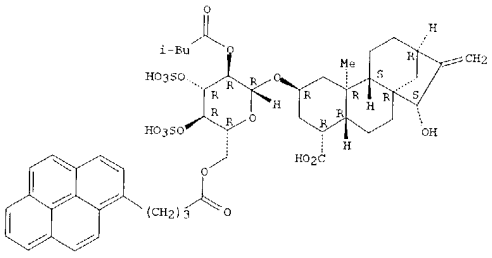
Absolute stereochemistry.



RN 267886-18-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-(1-oxo-4-(1-pyrenyl)butyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

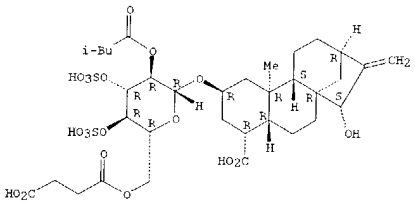
Absolute stereochemistry.

L20 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-21-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-(3-carboxy-1-oxopropyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



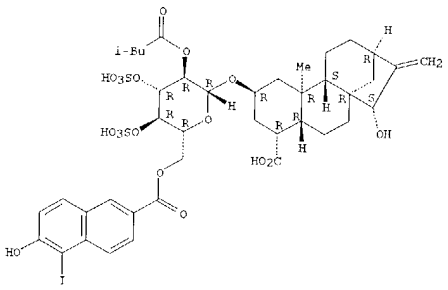
RN 267886-32-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L20 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 267886-38-4 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[(6-hydroxy-5-iodo-2-naphthalenyl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 267886-40-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-[[2-(4-hydroxy-3-iodophenyl)ethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L20 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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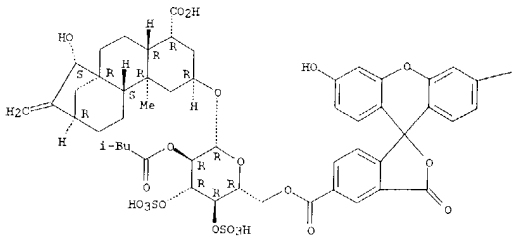

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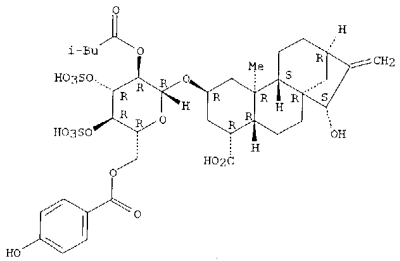
OH

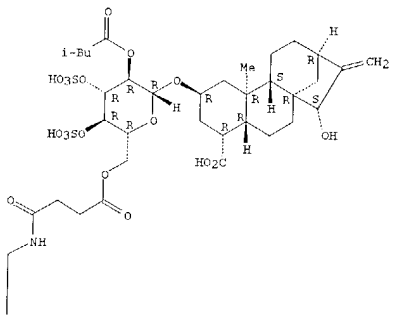
RN 267886-36-2 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-(4-hydroxybenzoyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L20 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



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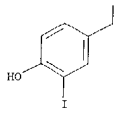
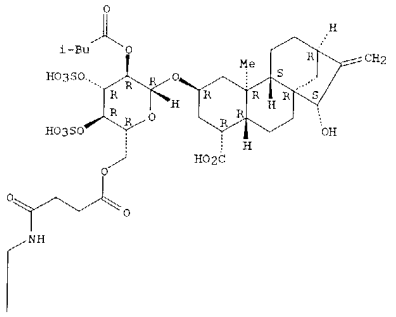


RN 267886-41-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-[[2-(4-hydroxy-3,5-diiodophenyl)ethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

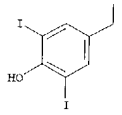
Absolute stereochemistry.

L20 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



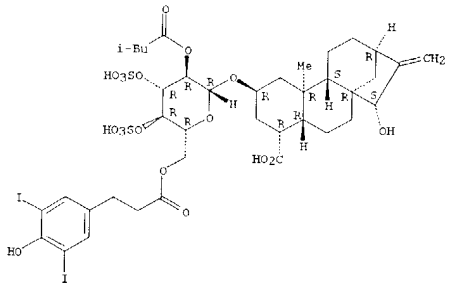
PAGE 2-A



RN 267886-42-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxy-3,5-diiodophenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

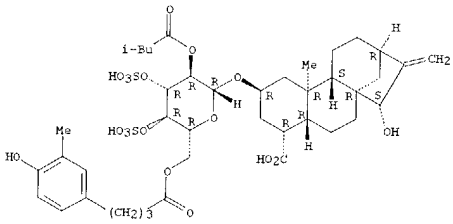
Absolute stereochemistry.

L20 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-43-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-(4-hydroxy-3-methylphenyl)-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

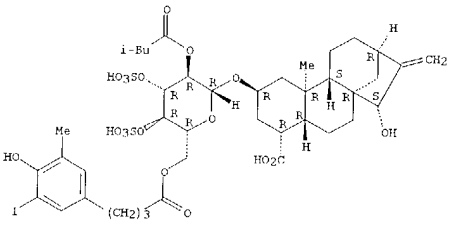
Absolute stereochemistry.



RN 267886-44-2 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-(4-hydroxy-3-iodo-5-methylphenyl)-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

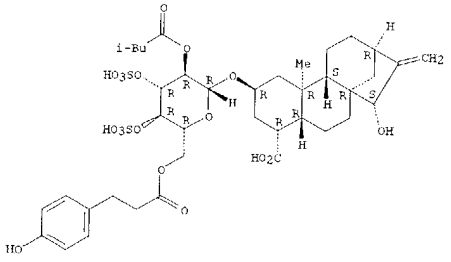
Absolute stereochemistry.

L20 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-45-3 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxyphenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

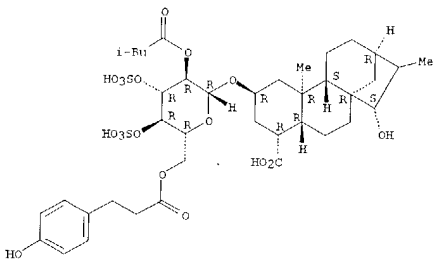
Absolute stereochemistry.



RN 267886-46-4 CAPLUS
CN 19-Norkauran-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxyphenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α,16ξ)- (9CI) (CA INDEX NAME)

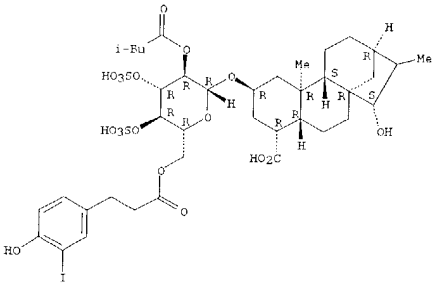
Absolute stereochemistry.

L20 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-47-5 CAPLUS
CN 19-Norkauran-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxy-3-iodophenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α,16ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L20 ANSWER 3 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:686759 CAPLUS
DOCUMENT NUMBER: 136:98644
TITLE: Fluorometric detection of ADP/ATP carrier deficiency in human muscle
AUTHOR(S): Fiore, C.; Arlot-Guilligay, D.; Trezeguet, V.; Lauquin, G. J.-M.; Brandolin, G.
CORPORATE SOURCE: Laboratoire de Biophysique et Biochimie des Systemes Integres, CEA-Grenoble, UMR 5092 CEA-CNRS-UJF, Grenoble, 38054, Fr.
SOURCE: Clinica Chimica Acta (2001), 311(2), 125-135
CODEN: CCATAR; ISSN: 0009-8981
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

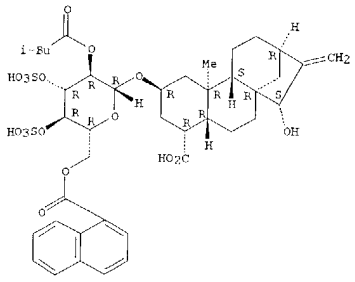
AB Defects in mitochondrial energy metabolism lead to severe disorders in humans
referred to as mitochondriocytopathies. Most of them have been reported to result from deficiencies of one or more complexes of the respiratory chain and, more rarely, from mitochondrial transmembrane metabolite carrier defects. Dysfunctioning of the ADP/ATP carrier, which catalyzes the export of matrix ATP in exchange for cytosolic ADP, has been demonstrated to induce myopathies in mouse and in humans. To screen for ADP/ATP carrier deficiency in patients suffering from mitochondriocytopathy with no defined etiol., we have set up a fluorometric assay to quantify the ADP/ATP carrier in small muscle homogenates, without preliminary isolation of mitochondria. The assay is based on the use of a fluorescent derivative of atractyloside, namely naphthoyl-atractyloside, a highly specific inhibitor of ADP/ATP transport. Here, we describe anal. of healthy and pathol. muscle samples, and characterization of ADP/ATP carrier deficiencies in two patients, one displaying an absence of the carrier and the second one containing a limited amount of the carrier with altered binding properties.

IT **84882-67-7**
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(fluorometric detection of ADP/ATP carrier deficiency in human muscle)

RN 84882-67-7 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-(1-naphthalenylcarbonyl)-2,3-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L20 ANSWER 3 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:314834 CAPLUS
DOCUMENT NUMBER: 132:344104
TITLE: Cloning and production of human adenine nucleotide translocator and the synthesis and screening assays for novel ligands
INVENTOR(S): Anderson, Christen M.; Davis, Robert E.; Clevenger, William; Wiley, Sandra Eileen; Miller, Scott W.; Szabo, Tomas R.; Ghosh, Soumitra S.
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 175 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000026370 | A2 | 20000511 | WO 1999-US25883 | 19991103 |
| WO 2000026370 | A3 | 20001116 | | |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1049780 | A1 | 20001108 | EP 1999-968032 | 19991103 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| JP 2002539761 | T2 | 20021126 | JP 2000-579742 | 19991103 |
| US 2001044144 | A1 | 20011122 | US 2001-811094 | 20010314 |
| US 2002012992 | A1 | 20020131 | US 2001-810644 | 20010314 |
| PRIORITY APPLN. INFO.: | | | US 1998-185904 A | 19981103 |
| | | | US 1999-393441 A | 19990908 |
| | | | WO 1999-US25883 W | 19991103 |

OTHER SOURCE(S): MARPAT 132:344104

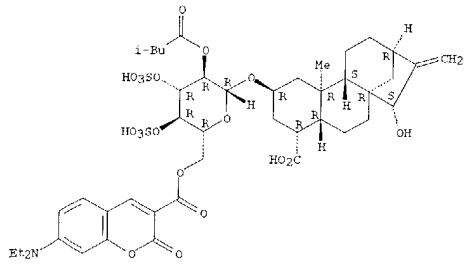
AB Compns. and methods are provided for producing adenine nucleotide translocator (ANT) polypeptides and fusion proteins, including the production
and use of recombinant expression constructs having a regulated promoter. Bacterial, insect, yeast (Sf9 cells and Trichoplusia ni cells), and mammalian expression systems are designed for reliable production of recombinant human ANT polypeptides in significant quantities, by employing regulated promoters and recombinant ANT fusion products with glutathione S-transferase and green fluorescent protein. The synthesis and properties of representative atractyloside derivs. as ANT ligands are described. ANT ligands and compns. and methods for identifying ANT ligands, agents that bind ANT, and agents that interact with ANT are also disclosed.

IT **267886-17-9P 267886-18-0P**
RL: ARG (Analytical reagent use); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(cloning and production of human adenine nucleotide translocator and the synthesis and screening assays for novel ligands)

RN 267886-17-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[[7-(diethylamino)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

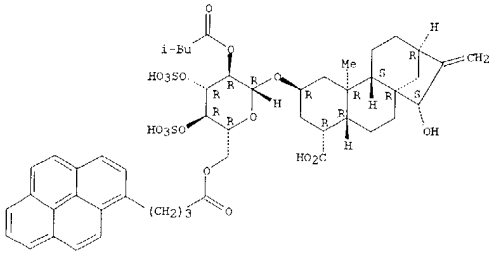
Absolute stereochemistry.

L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-18-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-[1-oxo-4-(1-pyrenyl)butyl]-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

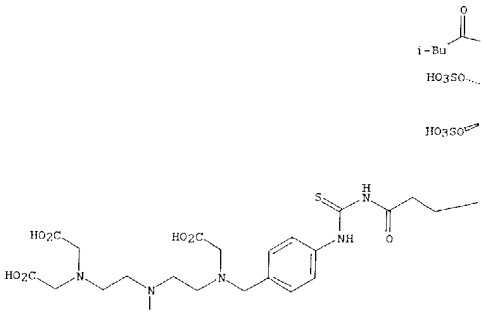


IT **267886-22-6P 267886-24-8P 267886-26-0P**
**267886-28-2P 267886-30-6P 267886-50-0P**
**267886-56-6P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(cloning and production of human adenine nucleotide translocator and the synthesis and screening assays for novel ligands)

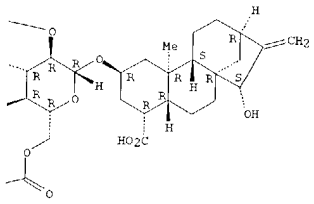
L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RN 267886-22-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[[[[4-[[[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl](carboxymethyl)amino]methyl]phenyl]amino]thioxomethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



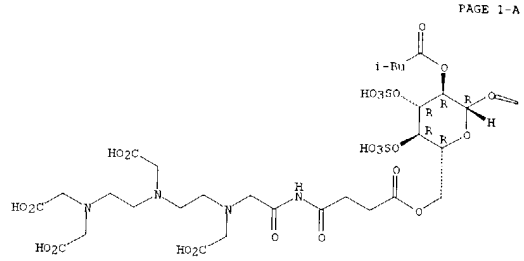
L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 2-A

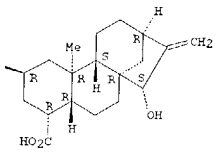
RN 267886-24-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[15-carboxy-8,11,14-tris(carboxymethyl)-1,4,6-trioxo-5,8,11,14-tetraazapentadec-1-yl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

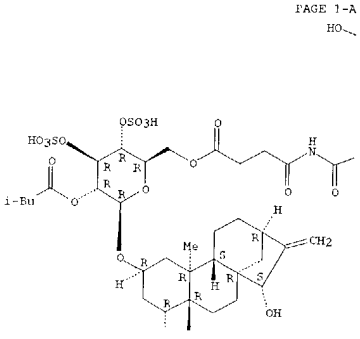


RN 267886-26-0 CAPLUS

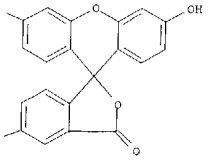
L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)carbonyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



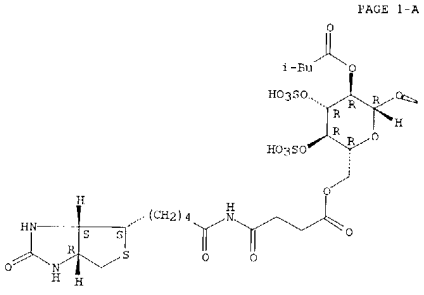
PAGE 2-A

RN 267886-28-2 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[[5-[(3aS,4S,6aR)-hexahydro-2-oxo-

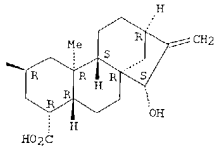
L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



RN 267886-30-6 CAPLUS
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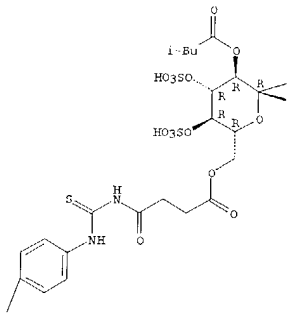
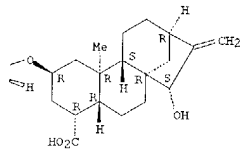
Absolute stereochemistry.

L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A

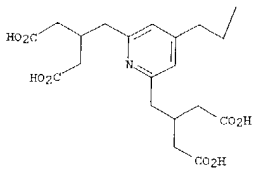


PAGE 1-B



L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

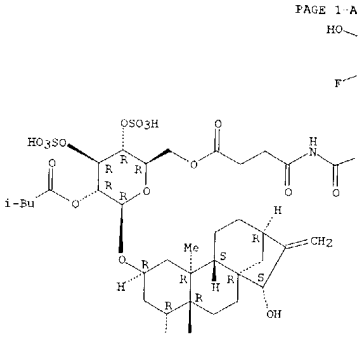
PAGE 2-A



RN 267886-50-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[[(2',7'-difluoro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)carbonyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4aα,15α)- (9CI) (CA INDEX NAME)

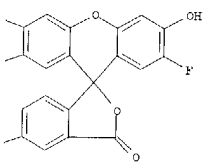
Absolute stereochemistry.

PAGE 1-A



L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-B



PAGE 2-A

RN 267886-56-6 CAPLUS
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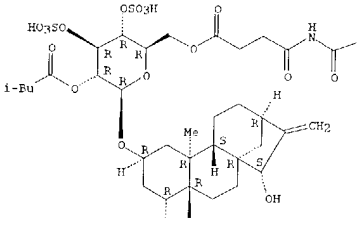
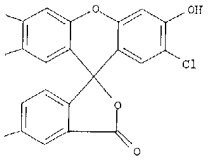
Absolute stereochemistry.

PAGE 1-A



L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-B



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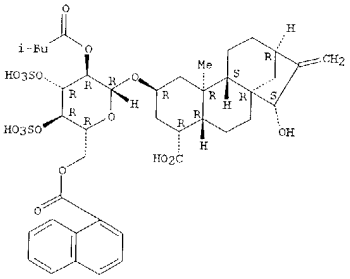
IT **84882-67-7P 267886-32-8P 267886-33-9P**
**267886-34-0P 267886-35-1P 267886-36-2P**
**267886-37-3P 267886-38-4P 267886-39-5P**
**267886-40-8P 267886-41-9P 267886-42-0P**
**267886-43-1P 267886-44-2P 267886-45-3P**
**267886-46-4P 267886-47-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(cloning and production of human adenine nucleotide translocator and the synthesis and screening assays for novel ligands)

RN 84882-67-7 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-(1-naphthalenylcarbonyl)-2,3-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4aα,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

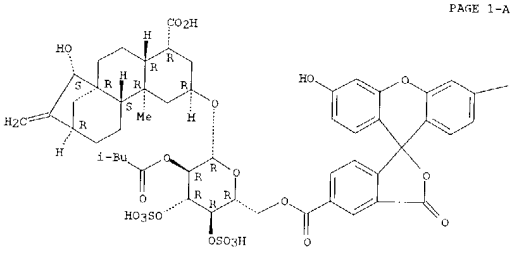
L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-32-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

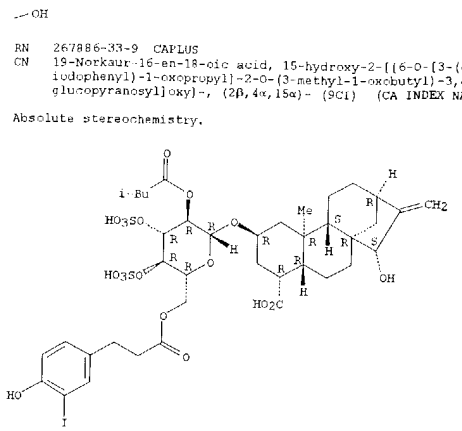
Absolute stereochemistry.

PAGE 1-A



L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-B



RN 267886-33-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxy-3-iodophenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

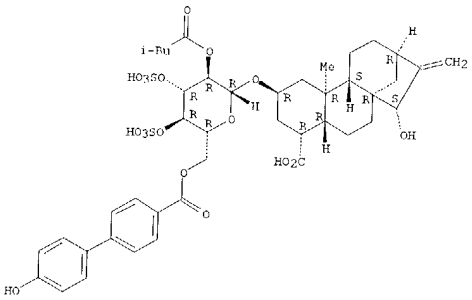
Absolute stereochemistry.



RN 267886-34-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[(4'-hydroxy[1,1'-biphenyl]-4-yl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-35-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[(4'-hydroxy-3'-iodo[1,1'-biphenyl]-4-yl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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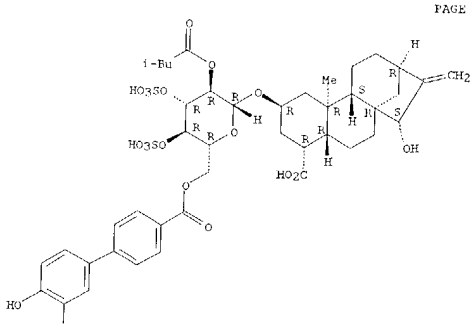
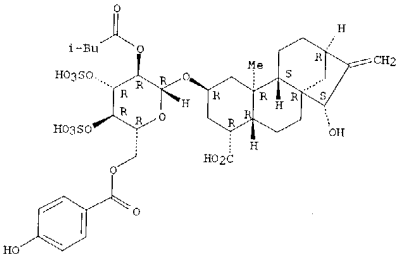


L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 2-A



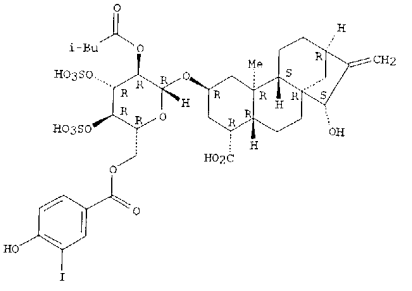
RN 267886-36-2 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-(4-hydroxybenzoyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 267886-37-3 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-(4-hydroxy-3-iodobenzoyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

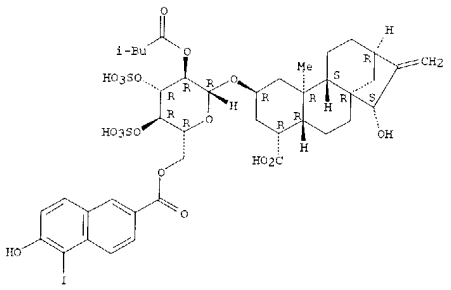
Absolute stereochemistry.



L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 267886-38-4 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[(6-hydroxy-5-iodo-2-naphthalenyl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 267886-39-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-[[2-(4-hydroxyphenyl)ethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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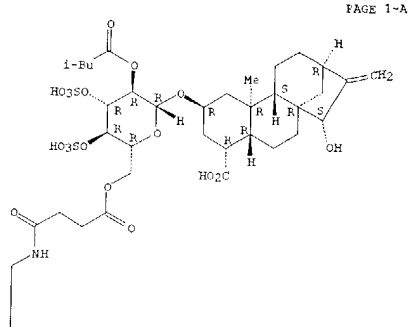
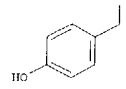


PAGE 2-A

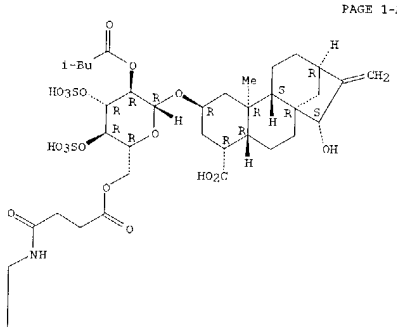


RN 267886-40-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-[[2-(4-hydroxy-3-iodophenyl)ethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

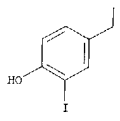
Absolute stereochemistry.

L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



PAGE 2-A

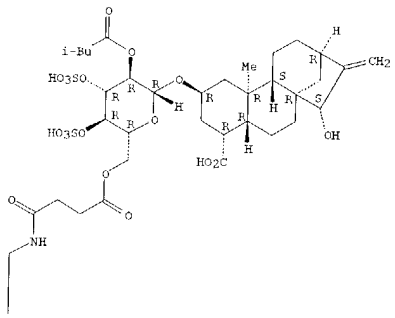


RN 267886-41-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-[[2-(4-hydroxy-3,5-diiodophenyl)ethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



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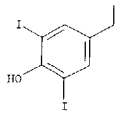
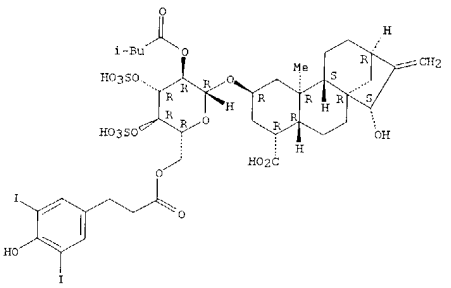


RN 267886-42-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxy-3,5-diiodophenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

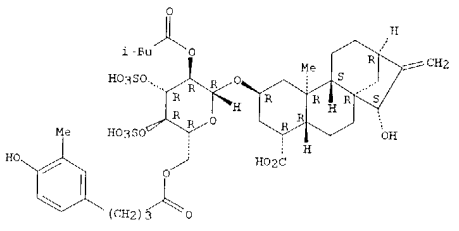
Absolute stereochemistry.

L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-43-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-(4-hydroxy-3-methylphenyl)-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

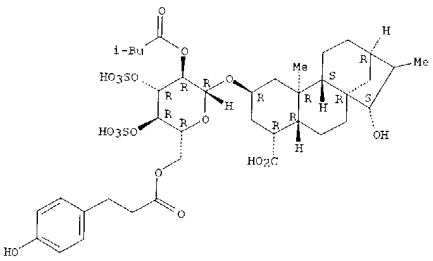
Absolute stereochemistry.



RN 267886-44-2 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[4-(4-hydroxy-3-iodo-5-methylphenyl)-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

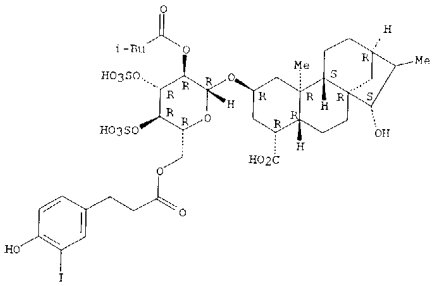
Absolute stereochemistry.

L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



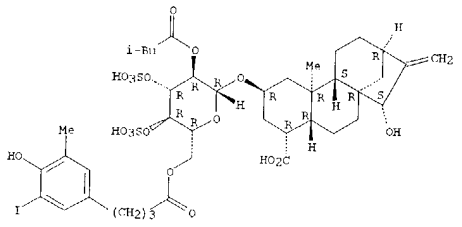
RN 267886-47-5 CAPLUS
CN 19-Norkauran-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxy-3-iodophenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α,16ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



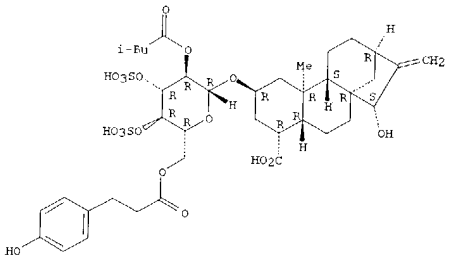
IT **267886-21-5DP**, alkyldiamine derivs. **267886-21-5P** **267886-53-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cloning and production of human adenine nucleotide translocator and the synthesis and screening assays for novel ligands)
RN 267886-21-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-(3-carboxy-1-oxopropyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-

L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 267886-45-3 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxyphenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

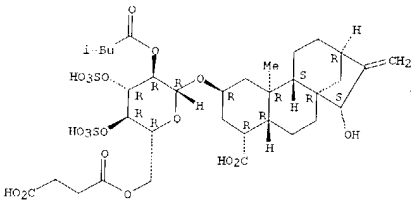


RN 267886-46-4 CAPLUS
CN 19-Norkauran-18-oic acid, 15-hydroxy-2-[[6-O-[3-(4-hydroxyphenyl)-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α,16ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

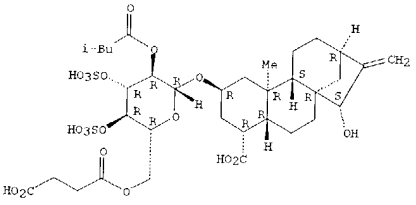
L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 267886-21-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-(3-carboxy-1-oxopropyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 267886-53-3 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[(4'-hydroxy-3',5'-diiodo[1,1'-biphenyl]-4-yl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L20 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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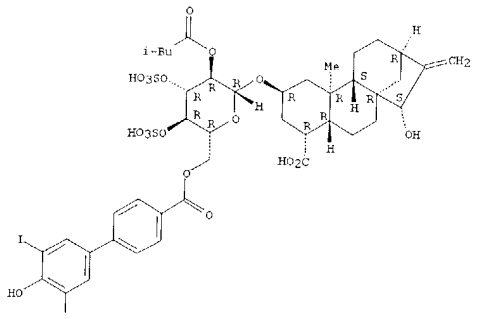

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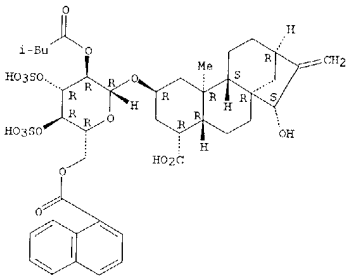
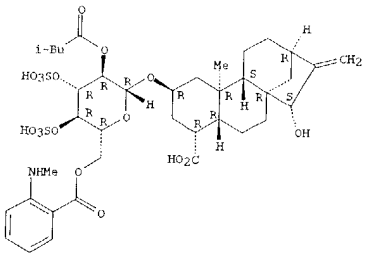
L20 ANSWER 5 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT **174584-83-9P**
RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(fluorometry of mitochondrial ADP/ATP carrier in muscle with atractyloside derivs.)
RN 174584-83-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[6-O-[2-(methylamino)benzoyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



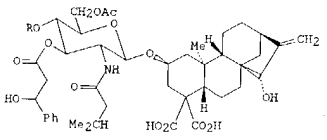
L20 ANSWER 5 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:96368 CAPLUS
DOCUMENT NUMBER: 124:225476
TITLE: Fluorometric titration of the mitochondrial ADP/ATP carrier protein in muscle homogenate with atractyloside derivatives
AUTHOR(S): Roux, Pierre; Le Saux, Agnes; Fiore, Christelle; Schwimmer, Christine; Dianoux, Anne-Christine; Trezeguet, Veronique; Vignais, Pierre V.; Lauquin, Guy J.-M.; Brandolin, Gerard
CORPORATE SOURCE: Laboratoire Biochimie, DBMS, Grenoble, 38054, Fr.
SOURCE: Analytical Biochemistry (1996), 234(1), 31-7
CODEN: ANBCA2; ISSN: 0003-2697
PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors describe the chemical synthesis of the novel methylanthraniloyl (Mant-) derivative of atractyloside (ATR), which is a specific inhibitor of the mitochondrial ADP/ATP carrier. The spectral properties of Mant-ATR and naphthoyl-ATR (N-ATR) are analyzed. Both derivs. bind to the membrane-bound ADP/ATP carrier at the same sites as ATR and carboxyatractyloside (CATR). When Mant-ATR and N-ATR are displaced by CATR, their fluorescence emissions are decreased and increased, resp. These fluorescence changes allow the titration of the CATR binding sites and therefore the quantitation of the amount of ADP/ATP carrier protein in a biol. preparation The validity of the fluorometric titration was tested with beef heart mitochondria and confirmed by binding assays using radioactive ATR. The fluorometric method was applied to rabbit skeletal muscle homogenate and the results of titration were confirmed by binding assays of radioactive ATR. The reliability of the fluorometric method was assessed by comparing the amts. of CATR binding sites and the content of heme aa3 in muscle homogenates and in isolated mitochondria from the same homogenates. Because of its high sensitivity, the fluorometric titration of the ADP/ATP carrier requires small amts. of tissue. Mant-ATR and N-ATR can therefore be considered as convenient, reliable, and sensitive probes to quantify the amount of ADP/ATP carrier and detect a putative carrier protein deficiency in biopsy samples from human patients suffering from myopathies with no clear identified etiol.

IT **84882-67-7**
RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)
(fluorometry of mitochondrial ADP/ATP carrier in muscle with atractyloside derivs.)
RN 84882-67-7 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-(1-naphthalenylcarbonyl)-2,3-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L20 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:20970 CAPLUS
DOCUMENT NUMBER: 114:20970
TITLE: Bifloratoxin, a toxic aminoglycoside of carboxyatractyligenin, from Melanthera biflora
AUTHOR(S): MacLeod, John K.; Gaul, Kim L.; Oelrichs, Peter B.
CORPORATE SOURCE: Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia
SOURCE: Australian Journal of Chemistry (1990), 43(9), 1533-9
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

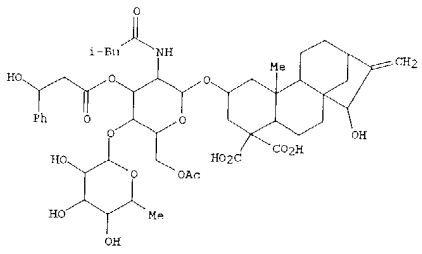


I, R=rhamosyl

AB The structure of the toxic kaurene aminoglycoside bifloratoxin (I) from M. biflora was determined, and complete 1H and 13C NMR spectral assignments achieved. The aglycon unit of I was identical to carboxyatractyligenin, the aglycon of carboxyatractyloside.

IT **131009-41-1**, Bifloratoxin
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Melanthera biflora, isolation and structure determination of)
RN 131009-41-1 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 2-[[6-O-acetyl-2-deoxy-4-O-(6-deoxy-α-L-mannopyranosyl)-3-O-(3-hydroxy-1-oxo-3-phenylpropyl)-2-[(3-methyl-1-oxobutyl)amino]-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,15α)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



L20 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

IT **131125-09-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 131125-09-2 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 2-[[6-O-acetyl-2-deoxy-4-O-[6-deoxy-2,3,4-tris-O-(trimethylsilyl)-α-L-mannopyranosyl]-2-[(3-methyl-1-oxobutyl)amino]-3-O-[1-oxo-3-phenyl-3-[(trimethylsilyl)oxy]propyl]-β-D-glucopyranosyl]oxy]-15-[(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester, (2β,15α)- (9CI) (CA INDEX NAME)

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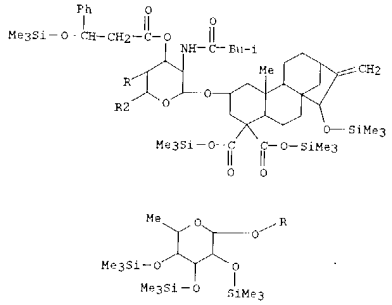

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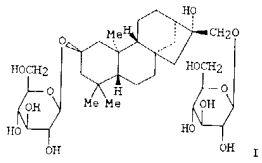
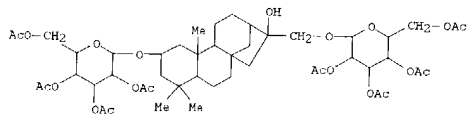
L20 ANSWER 7 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:218947 CAPLUS
DOCUMENT NUMBER: 108:218947
TITLE: The characterization of a diterpene diglycoside from Jamaican Turbina corymbosa. Application of 2D NMR in its structure determination
AUTHOR(S): Nair, Muraleedharan G.; Burke, Basil A.; Manning, Kenneth S.; Lynn, David G.
CORPORATE SOURCE: Dep. Chem., Univ. West Indies, Kingston, Jamaica
SOURCE: Journal of Chemical Research, Synopses (1987), (10), 318-19
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

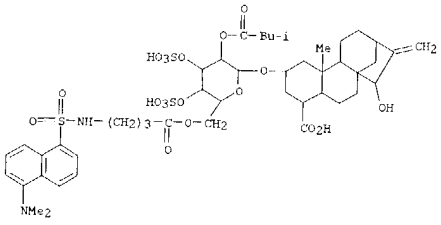


I

AB A new diterpene diglycoside (I) was shown to be a major constituent in seeds of T. corymbosa. The structure of I was determined by spectral methods.
IT **114590-51-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 114590-51-1 CAPLUS
CN β-D-Glucopyranoside, (2β)-16-hydroxykaurane-2,17-diyl bis-, 2,2',3,3',4,4',6,6'-octaacetate (9CI) (CA INDEX NAME)



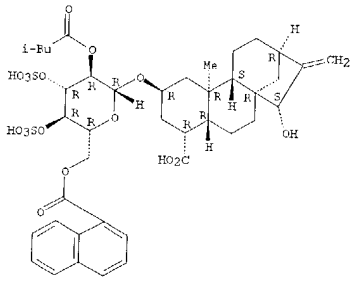
L20 ANSWER 8 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1986:530300 CAPLUS
DOCUMENT NUMBER: 105:130300
TITLE: Fluorescent probes of the mitochondrial ADP/ATP carrier protein
AUTHOR(S): Block, Marc R.; Boulay, Francois; Brandolin, Gerard; Dupont, Yves; Lauquin, Guy J. M.; Vignais, Pierre V.
CORPORATE SOURCE: Dep. Rech. Fundamen., Cent. Etudes Nucl., Grenoble, 38041, Fr.
SOURCE: Methods in Enzymology (1986), 125(Biomembranes, Pt. M), 639-49
CODEN: MENZAU; ISSN: 0076-6879
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Fluorescent probes of the ADP/ATP-carrier protein (I) include naphthoyl-ADP and naphthoyl-ATP, and atractyloside (ATR) derivs., dansyl-ATR, dansyl-4-aminobutyryl-ATR and naphthoyl-ATR. The preparation and use of these compds. in the determination and conformational anal. of I are described.
IT **84872-88-8 84882-67-7**
RL: ANST (Analytical study)
(as fluorescent probe, of adenine nucleotide-transporting protein)
RN 84872-88-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)



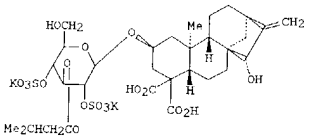
RN 84882-67-7 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-(1-naphthalenylcarbonyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L20 ANSWER 8 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L20 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1983:435952 CAPLUS
DOCUMENT NUMBER: 99:35952
TITLE: Atractylosides in Callilepis laureola (Asteraceae)
AUTHOR(S): Brookes, K. Bridget; Candy, H. Arthur; Pegel, Karl H.
CORPORATE SOURCE: Dep. Chem., Univ. Durban-Westville, Durban, S. Afr.
SOURCE: South African Journal of Chemistry (1983), 36(2), 65-8
CODEN: SAJCDG; ISSN: 0379-4350
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

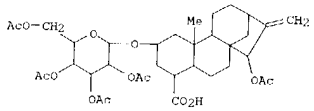


I

AB In addition to the previously reported atractyloside, 3 more kaurenoid glucosides were found in the root-stock of C. laureola. These are carboxyatractyloside (I) and the 6'-isovaleryl esters of atractyloside and carboxyatractyloside. This is the first report of the 2 6'-isovalerates. The β-glucosidic nature of these poisonous Asteraceae atractylosides was confirmed by 1H and 13C NMR, spectroscopic and mol. rotation evidence.

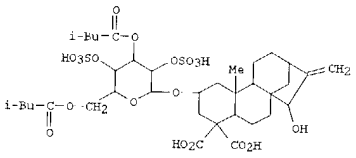
IT **61773-42-0 61773-43-1 86368-84-5 86368-85-6**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Callilepis laureola)

RN 61773-42-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-(acetyloxy)-2-[[2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)



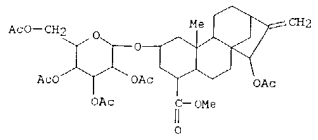
RN 61773-43-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-(acetyloxy)-2-[[2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl]oxy]-, methyl ester, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L20 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

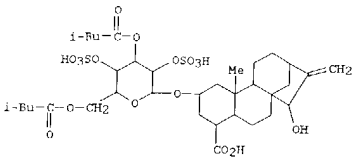


●2 K

L20 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 86368-84-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[2,6-bis-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)



●2 K

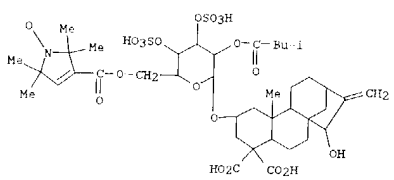
RN 86368-85-6 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 2-[[2,6-bis-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,15α)- (9CI) (CA INDEX NAME)

L20 ANSWER 10 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1983:139309 CAPLUS
DOCUMENT NUMBER: 98:139309
TITLE: Binding of spin-labeled carboxyatractylate to mitochondrial adenosine 5'-diphosphate/adenosine 5'-triphosphate carrier as studied by electron spin resonance
AUTHOR(S): Munding, Anton; Beyer, Klaus; Klingenberg, Martin
CORPORATE SOURCE: Inst. Physiol. Chem., Univ. Muenchen, Munich, 8000/2, Fed. Rep. Ger.
SOURCE: Biochemistry (1983), 22(8), 1941-7
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

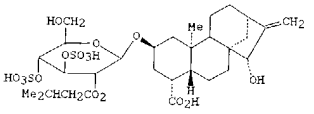
AB The spin-label 2,2,5,5-tetramethyl-1-oxy-3-pyrroline-3-carboxylic acid was attached to the inhibitor carboxyatractylate of the mitochondrial ADP/ATP carrier (adenine nucleotide translocase). Being closely linked to the inhibitor, the spin-label should reflect the mobility of the carboxyatractylate. When bound to the carrier in mitochondria, spin-labeled carboxyatractylate reveals a most unusual hyperfine splitting of 72 G. A 2nd spectral component with a hyperfine splitting of 62 G is also mainly due to carrier-bound inhibitor. A similar spectrum with somewhat reduced hyperfine splitting was observed with the detergent-solubilized protein, whereas reincorporation into phospholipid membranes yielded almost the same spectra as in mitochondria. The carrier-bound spin-label is concluded to be highly immobilized. The less immobilized spectral component is discussed in terms of strongly anisotropic label motion. In addition, the unusual splitting is interpreted to indicate the highly polar environment of the nitroxide. The interpretations are supported by the temperature dependence, which indicates a reversible progressive spin-label mobilization up to 50°. Membrane-impermeable reducing agents showed that the spin-label is easily accessible from the aqueous phase.

IT **84602-22-2**
RL: PROC (Process)
(adenine nucleotide translocase binding of)

RN 84602-22-2 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 1-[[6-O-[(2,5-dihydro-2,2,5,5-tetramethyl-1-oxy-1H-pyrrol-3-yl)carbonyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,15α)- (9CI) (CA INDEX NAME)



L20 ANSWER 11 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1983:103893 CAPLUS
DOCUMENT NUMBER: 98:103893
TITLE: Synthesis and properties of fluorescent derivatives of atractyloside as potential probes of the mitochondrial ADP/ATP carrier protein
AUTHOR(S): Boulay, Francois; Brandolin, Gerard; Lauquin, Guy J. M.; Vignais, Pierre V.
CORPORATE SOURCE: Dep. Rech. Fondam., Cent. Etudes Nucl., Grenoble, 38041, Fr.
SOURCE: Analytical Biochemistry (1983), 128(2), 323-30
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



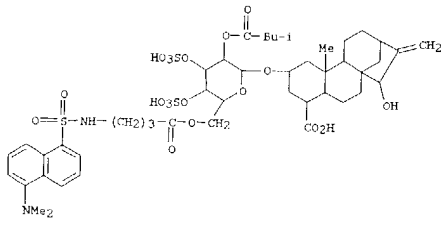
I

AB The chemical synthesis of fluorescent derivs. of atractyloside (I) (ATR), an inhibitor of the mitochondrial ADP/ATP carrier protein, is described. These derivs. are: 6'-O-dansyl-ATR; 6'-O-dansyl-aminobutyryl-ATR; and 6'-O-naphthoyl-ATR. The spectral properties of these analogs were analyzed, and their biol. features were compared to those of ATR. The fluorescence emission of the dansyl-ATR derivs. was increased in organic solvents and that of naphthoyl-ATR was decreased; for both analogs, solubilization in organic solvents resulted in a blue shift of the emission peak. The fluorescent dansyl- and naphthoyl-ATR derivs. were specifically recognized by the mitochondrial ADP/ATP carrier protein. Because of their spectral properties and their biochem. reactivities, the fluorescent analogs of ATR can be considered as potential probes to investigate the topog. of the ADP/ATP carrier in the mitochondrial membrane and to monitor conformational changes of the ADP/ATP carrier protein associated with transport.

IT **84872-88-8P 84882-67-7P**
RL: PREP (Preparation)
(preparation of, as mitochondrial ADP/ATP carrier protein probe)

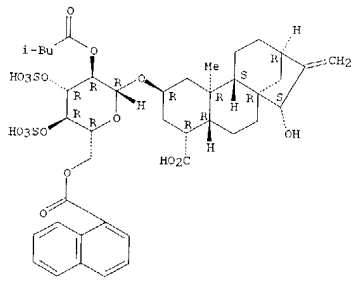
RN 84872-88-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L20 ANSWER 11 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 84882-67-7 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-(1-naphthalenylcarbonyl)-2,3-di-O-sulfo-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



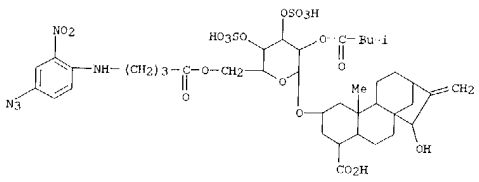
L20 ANSWER 12 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1983:49494 CAPLUS
DOCUMENT NUMBER: 98:49494
TITLE: Photolabeling approach to the study of the topography of the atractyloside binding site in mitochondrial adenosine 5'-diphosphate/adenosine 5'-triphosphate carrier protein
AUTHOR(S): Boulay, Francois; Lauquin, Guy J. M.; Tsugita, Akira; Vignais, Pierre V.
CORPORATE SOURCE: Dep. Rech. Fondam., Cent. Etud. Nucl., Grenoble, Fr.
SOURCE: Biochemistry (1983), 22(2), 477-84
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The binding site of atractyloside (I), an impermeant inhibitor of the mitochondrial ADP/ATP carrier protein (adenine nucleotide translocase) (II), was investigated by photolabeling techniques. The photolabels used were long- and short-arm radioactive derivs. of I, namely, 6'-O-[3-[N-(4-azido-2-nitrophenyl)amino]propionyl]-I, 6'-O-[4-[N-(4-azido-2-nitrophenyl)amino]butyryl]-I, and 6'-O-(p-azidobenzoyl)-I. The photolabeling step was carried out with bovine heart mitochondria. Covalently photolabeled II was extracted by Triton X-100 and further purified by hydroxylapatite chromatog., acetone precipitation, and washing with a mixture of formic acid, EtOH, and ether. The peptide chain was cleaved at methionine and cysteine residues by specific chemical reagents. Cleavage of II (mol. weight 32,000) at the methionine residues by CNBr yielded a large, 23,000-dalton segment, called CB1, that was radiolabeled and a number of unlabeled small fragments. Cleavage at cysteinyl residues by cyanide at alkaline pH involved the prior reaction of SH groups with 5,5'-dithiobis(2-nitrobenzoic acid). Cyanide cleavage of the CB1 fragment, which contains 3 cysteinyl residues, resulted in the accumulation of a number of overlapping peptides and 4 nonoverlapping peptides, these latter being referred to as CN peptides. With both the long- and short-arm azido-I derivs. used, essentially only 1 of the CN peptides, with a mol. weight of .apprx.4500, was found to be photolabeled; this peptide was situated at the C-terminus of the CB1 fragment between cysteine-159 and methionine-200. Thus, the I site in membrane-bound II is located near the center of mol.; this region may be exposed to the cytosolic side of the inner mitochondrial membrane.

IT **65792-55-4 83876-80-6 83876-82-8**
RL: BIOL (Biological study)
(adenine nucleotide translocase photolabeling by, atractyloside-binding site in relation to)

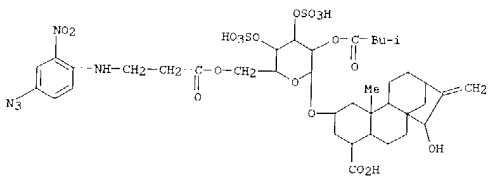
RN 65792-55-4 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[(4-azido-2-nitrophenyl)amino]-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L20 ANSWER 12 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 K

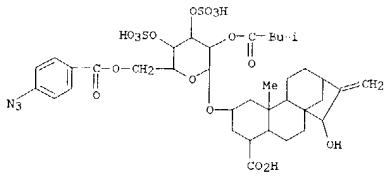
RN 83876-80-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[3-[(4-azido-2-nitrophenyl)amino]-1-oxopropyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)



●2 K

RN 83876-82-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-(4-azidobenzoyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L20 ANSWER 12 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 K

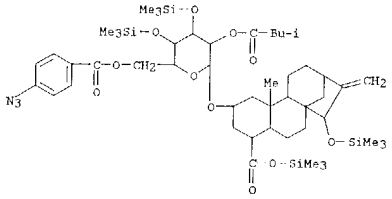
L20 ANSWER 13 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:595352 CAPLUS
DOCUMENT NUMBER: 97:195352
TITLE: Synthesis of 6'-O-p-azidobenzoylatractyloside, a short arm photoactivable derivative of atractyloside. Studies of its binding and inhibitory properties
AUTHOR(S): Boulay, Francois; Lauquin, Guy J. M.; Vignais, Pierre V.
CORPORATE SOURCE: Lab. Biochim., CNRS/EHA, Grenoble, 38041, Fr.
SOURCE: FEBS Letters (1982), 143(2), 268-72
CODEN: FEBLAL; ISSN: 0014-5793
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis of a radiolabeled short-arm photoactivable derivative of atractyloside (I), 6'-O-p-azido[14C]benzoylatractyloside (II), is described, as well as its spectral properties and reversible binding to the ADP/ATP carrier protein in rat heart mitochondrial membrane. For the synthesis of II, p-amino[14C]benzoic acid was diazotized to give p-azido[14C]benzoic acid (III) which then was coupled to I following activation of the carboxyl group of III by N,N'-carbonyldiimidazole. Following removal of unreacted III, the residue was dissolved in MeOH and subjected to reversed-phase high-pressure liquid chromatog. in a μBondapack C18 column equipped with a CO-pell ODS guard column and isocratic elution with MeOH-NH4OAc-HOAc-H2O (58:1:1:40). The effluent contained a main product which was identified as II by mass spectrometry and whose purity was assessed by TLC. The absorption spectra of II and photolysis by UV irradiation were examined Reversible binding of II in the dark to the ADP/ATP carrier protein in the mitochondrial membrane and competitive inhibition of ADP transport in rat liver mitochondria by II indicated that II is recognized by the carrier with the same affinity and specificity as I itself.

IT **83579-67-3**
RL: PRP (Properties)
(mass spectrum of)

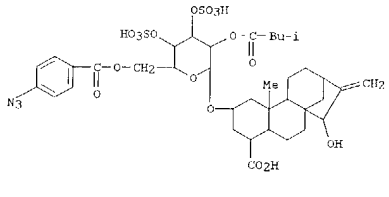
RN 83579-67-3 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-(4-azidobenzoyl)-2-O-(3-methyl-1-oxobutyl)-3,4-bis-O (trimethylsilyl)-β-D-glucopyranosyl]oxy]-15-[(trimethylsilyl)oxy]-, trimethylsilyl ester, (2β,4α,15α)- (9CI) (CA INDEX NAME)



L20 ANSWER 13 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

IT **83579-68-4P**
RL: PRP (Properties); PREP (Preparation)
(preparation and properties of, binding to ADP/ATP carrier protein of heart mitochondria membrane in relation to)

RN 83579-68-4 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-(4-azidobenzoyl)-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, labeled with carbon-14, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)



●2 K

L20 ANSWER 14 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN

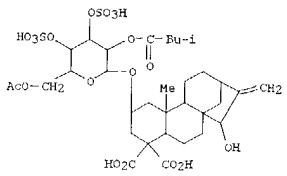
ACCESSION NUMBER: 1982:577110 CAPLUS
DOCUMENT NUMBER: 97:177110
TITLE: Interaction of naphthoyl-ADP a fluorescent ADP analog, with the ADP/ATP carrier protein in the mitochondrial membrane
AUTHOR(S): Block, Marc R.; Lauquin, Guy J. M.; Vignais, Pierre V.
CORPORATE SOURCE: Fac. Med., CEN/Grenoble, Grenoble, 38041, Fr.
SOURCE: Biochemistry (1982), 21(22), 5451-7
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 3'-O-(1-Naphthoyl ADP (N-ADP), a fluorescent analog of ADP, was established as a potent inhibitor of ADP/ATP transport in mitochondria and inside-out sonic particles; the Ki value was .apprx.5 μM. The inhibition was of a mixed type. On the other hand, N-ADP was not transported in a measurable way in either type of particles. Upon binding to the particles, the fluorescent intensity of N-ADP was decreased; the release of the bound N-ADP upon addition of carboxyatractyloside (CATR) to mitochondria and bongkrekic acid (BA) to sonic particles was reflected by increases of fluorescence. In parallel assays specifically bound [14C]N-ADP was equated to [14C]N-ADP released upon addition of either CATR (mitochondria) or BA (sonic particles). The specific binding of N-ADP corresponded to 1.4-1.6 nmol/mg of protein in mitochondria, with a Kd value of 3 μM, and to 1.5-1.6 nmol/mg of protein in sonic particles, with a Kd value of 6 μM. Similar values were obtained for N-ATP binding. These values are at least twice as high as those found for specific ADP or ATP binding, suggesting that N-ADP or N-ATP binds to potential nucleotide binding sites that were not totally occupied by ADP or ATP. Whereas nearly all the specifically bound N-ADP in mitochondria was displaced by an excess of ADP (400 μM) at pH 7.4, only 30% could be removed from sonic particles under the same conditions. Further at pH 6.5, ≤1/2 of the specifically bound N-ADP could be removed by excess ADP in mitochondria and only 10-20% in sonic particles. These results indicate that each ADP/ATP carrier unit contains ≥2 types of nucleotide sites capable of interacting with N-ADP. Because of the hydrophobic nature of the naphthoyl moiety of N-ADP, the data suggest that differences in N-ADP binding in mitochondria and sonic particles are related to differences in the hydrophobic nature of their sites. Inactivation studies were carried out with mitochondria and sonic particles to compare the sensitivity to UV light and butanedione of the binding of N-ADP, [3H]BA, and [14C]Ac-CATR, a radiolabeled substitute for CATR. Both in mitochondria and in sonic particles, UV light and butanedione more rapidly inactivated the binding of N-ADP than that of [3H]BA. However, in mitochondria, UV light more rapidly inactivated the binding of [14C]Ac-CATR than that of N-ADP; the reverse was true for the inactivation by butanedione. The inactivation data conclusively indicate that BA, CATR, and adenine nucleotides are recognized by different specific sets of amino acids.

IT **83103-09-7**
RL: BIOL (Biological study)
(adenine nucleotide transporter of mitochondria binding of, naphthoyl-ADP in comparison with)

RN 83103-09-7 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 2-[[6-O-acetyl-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,15α)- (9CI) (CA INDEX NAME)

L20 ANSWER 14 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 K

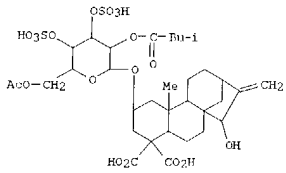
L20 ANSWER 15 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1980:581175 CAPLUS
DOCUMENT NUMBER: 93:181175
TITLE: Chemical radiolabeling of carboxyatractyloside by [14C]-acetic anhydride. Binding properties of [14C]-acetylcarboxyatractyloside to the mitochondrial ADP/ATP carrier
AUTHOR(S): Block, Marc R.; Pougeois, Richard; Vignais, Pierre V.
CORPORATE SOURCE: Dep. Rech. Fondamentale, CEN, Grenoble, 38041, Fr.
SOURCE: FEBS Letters (1980), 117(1), 335-40
CODEN: FEBLAL; ISSN: 0014-5793
DOCUMENT TYPE: Journal
LANGUAGE: English

AB [14C]acetylcarboxyatractyloside (I) was virtually identical to carboxyatractyloside (CAT) in binding to the mitochondrial ADP/ATP carrier. I bound to specific sites of the outer membrane of the carrier with an affinity constant (Kd) of 2-10 μM and irreversibly inhibited ADP/ATP transport. I was replaced by CAT but not by atractyloside and the I-carrier complex was stable after solubilization. I, in double-labeling expts. with [3H]bongkrekic acid (BA), showed mutual exclusion of CAT and BA mitochondrial binding sites. This exclusion was dependent on exptl. conditions. Further, addition of ADP + I during the pre-labeling step resulted in a much lower release of I on BA addition than when ADP + BA were added during the displacement step. This is probably related to different conformations of the carrier. A preparative method for I is given.

IT **75240-94-7**
RL: BIOL (Biological study)
(mitochondrial ADP-ATP carrier binding and inhibition by)

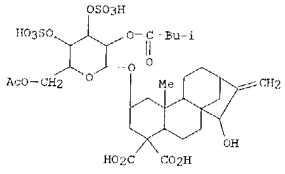
RN 75240-94-7 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 2-[[6-O-acetyl-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,15α)- (9CI) (CA INDEX NAME)



IT **75240-95-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 75240-95-8 CAPLUS
CN Kaur-16-ene-18,19-dioic acid, 2-[[6-O-acetyl-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, labeled with carbon-14, (2β,15α)- (9CI) (CA INDEX NAME)

L20 ANSWER 15 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



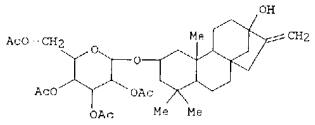
L20 ANSWER 16 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1980:528747 CAPLUS
DOCUMENT NUMBER: 93:128747
TITLE: Chemical and chemotaxonomic studies of Filices. Part XXVI. Chemical studies on the constituents of Lindsaea chienii Ching
AUTHOR(S): Satake, Toshiko; Murakami, Takao; Saiki, Yasuhisa; Chen, Chiu-Ming
CORPORATE SOURCE: Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1980), 28(6), 1859-63
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: German

AB From the aerial parts of L. chienii, a new diterpenoid glycoside (lindokaurenoside C) was isolated, together with lindsaea acid, creticoside, A, trans-cinnamic acid, and p-hydroxy-trans-cinnamic acid. From spectroscopic evidence and chemical reactions, the structure of the new glucoside has been established as ent-2α,13-dihydroxy-kaura-16-ene 2-O-β-D-glucoside.

IT **74730-18-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

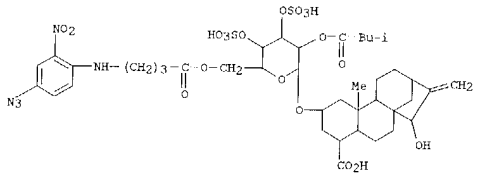
RN 74730-18-0 CAPLUS
CN β-D-Glucopyranoside, (2β)-13-hydroxykaur-16-en-2-yl, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)



L20 ANSWER 17 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1980:123624 CAPLUS
DOCUMENT NUMBER: 92:123624
TITLE: Fragmentation of the ADP/ATP carrier protein from beef heart mitochondria. Localization of the atractyloside binding site in a peptide obtained by cyanogen bromide cleavage
AUTHOR(S): Boulay, Francois; Lauquin, Guy J. M.; Vignais, Pierre V.
CORPORATE SOURCE: Dep. Rech. Fondam., CEN, Grenoble, 38041, Fr.
SOURCE: FEBS Letters (1979), 108(2), 390-4
CODEN: FEBLAL; ISSN: 0014-5793
DOCUMENT TYPE: Journal
LANGUAGE: English

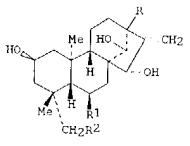
AB The atractyloside bind site of the ATP/ADP carrier protein of beef heart mitochondria was localized by photolabeling intact mitochondria with the nonpenetrant inhibitor N-4-azido-2-nitrophenylaminobutyryl atractyloside-3H (I), followed by extraction and purification of the photolabeled carrier and identification of the 3H-labeled peptide moiety following CNBr cleavage. CNBr cleavage products of the labeled purified protein were separated by column chromatog. and Na dodecyl sulfate-polyacrylamide gel electrophoresis. The 3H-labeled product consisted of a single 23,000-mol.-weight product which was homogeneous on gel electrophoresis. Amino acid anal. showed the polarity index of this product to be the same as that of the intact carrier (40%) and that the fragment and the intact carrier have the same blocked N-terminal amino acid residue in common. As I does not penetrate the mitochondrial membrane, at least part of the 23,000-mol.-weight fragment corresponds to the outer domain of the carrier protein and ≥1 region of this domain constitutes the atractyloside binding site. This domain is, hence, on the cytosol-exposed surface in the mitochondrial membrane. Studies with arylazido ADP indicated that ADP and atractyloside may bind to closely related sites on the carrier.

IT **73062-49-4**
RL: BIOL (Biological study)
(adenine nucleotide carrier binding site for, of mitochondrial membrane)
RN 73062-49-4 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[(4-azido-2-nitrophenyl)amino]-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)



L20 ANSWER 17 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

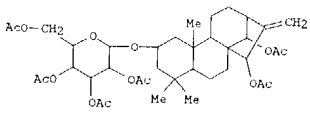
L20 ANSWER 18 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1979:69084 CAPLUS
DOCUMENT NUMBER: 90:69084
TITLE: Chemical and chemotaxonomical studies of the Pteris family and related families (Pteridaceae), XXI. Chemical studies of the contents of Pteris plumbaea Christ
AUTHOR(S): Tanaka, Nobutoshi; Nakatani, Kayoko; Murakami, Takao; Saiki, Yasuhisa; Chen, Chiu-Ming
CORPORATE SOURCE: Inst. Pharm., Agric. Univ. Tokyo, Tokyo, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1978), 26(10), 3260-4
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



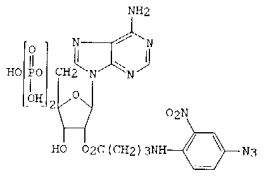
I, R=R1=R2=H
II, R=OH, R1=R2=H
III, R=R2=H, R1=OH
IV, R=R1=H, R2=OH

AB The previously known ent-kaurane derivs. creticoside A and ent-2α,14α,15β,16S,17-pentahydroxykaurane were isolated from the aerial parts of P. plumbaea by silica gel column chromatog. along with the 5 new kauranes named pterokaurane P1 (I), pterokaurane P2 (II), pterokaurane P3 (III), pterokaurane P4 (IV), and I 2-O-β-D-glucoside. Phys. and spectral data for each new compound is presented.

IT **69121-67-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 69121-67-1 CAPLUS
CN β-D-Glucopyranoside, (2β,14R,15α)-14,15-bis(acetyloxy)kaur-16-en-2-yl, tetraacetate (9CI) (CA INDEX NAME)



L20 ANSWER 19 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:100435 CAPLUS
DOCUMENT NUMBER: 88:100435
TITLE: Photoaffinity labeling of the adenine nucleotide carrier in heart and yeast mitochondria by an arylazido ADP analog
AUTHOR(S): Lauquin, Guy J. M.; Brandolin, Gerard; Lunardi, Joel; Vignais, Pierre V.
CORPORATE SOURCE: Dep. Rech. Fondam., CEN, Grenoble, Fr.
SOURCE: Biochimica et Biophysica Acta (1978), 501(1), 10-19
CODEN: BBACAQ; ISSN: 0006-3002
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

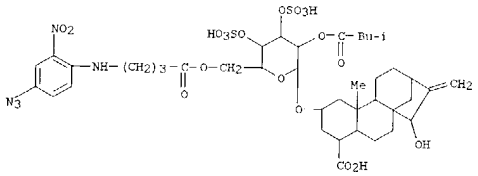


I

AB Arylazido analogs of ADP and ATP (N-4-azido-2-nitrophenylaminobutyryl-ADP (I) and N-4-azido-2-nitrophenylaminobutyryl-ATP) were prepared in radioactive form and used in photolabeling expts. to identify the adenine nucleotide carrier in mitochondria and sonic submitochondrial particles. When added in the dark to beef heart mitochondria, I bound to the adenine nucleotide carrier. I was not transported across the membrane to the matrix space, but did inhibit ADP transport in mitochondria. The inhibition was of a mixed type with a Ki value of .apprx. 10 μM. The nitrene derivative formed on photoirradn. of tritiated I bound to a polypeptide of apparent mol. weight 30,000 in beef heart mitochondria and 37,000 in Saccharomyces cerevisiae mitochondria. Photolabeling was prevented by preincubation of the mitochondria with atractyloside or carboxyatractyloside. Photoirradn. of sonic submitochondrial particles from beef heart (inside-out particles) with tritiated I resulted in the labeling of the 30,000-dalton polypeptide and also in the labeling of higher-mol.-weight peptides (50,000-55,000) probably belonging to F1 ATPase. Addition of bongkrekic acid specifically decreased the photolabeling of the 30,000-dalton polypeptide. An arylazido derivative of atractyloside (N-4-azido-2-nitrophenylaminobutyryl-atractyloside) bound on photoirradn. to the 30,000-dalton polypeptide in beef heart mitochondria and to the 37,000-dalton polypeptide in S. cerevisiae mitochondria. Since the adenine nucleotide carrier is readily damaged by UV light, nitroarylazido analogs of ADP and ATP or of atractyloside, which are photoactivated in visible light, were used in preference to other azido analogs, which require UV light for photoactivation. Thus, the same mitochondrial protein belonging to the adenine nucleotide transport system is able to bind ADP (or ATP) and atractyloside.

IT **65792-55-4**

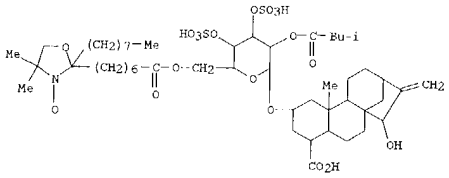
L20 ANSWER 19 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RL: BIOL (Biological study)
(photoaffinity labeling of adenine nucleotide carrier of mitochondria by)
RN 65792-55-4 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[(4-azido-2-nitrophenyl)amino]-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)



●2 K

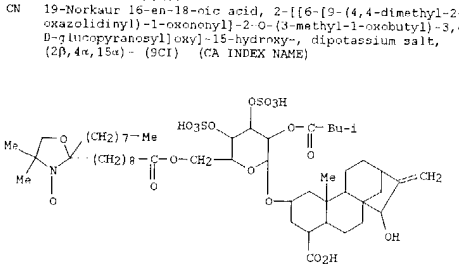
L20 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:166506 CAPLUS
DOCUMENT NUMBER: 86:166506
TITLE: Spin-labeled acyl atractyloside as a probe of the mitochondrial adenosine diphosphate carrier. Asymmetry of the carrier and direct lipid environment
AUTHOR(S): Lauquin, Guy J. M.; Devaux, Philippe F.; Bienvenue, Alain; Villiers, Christian; Vignais, Pierre V.
CORPORATE SOURCE: Dep. Rech. Fondam., CEN, Grenoble, Fr.
SOURCE: Biochemistry (1977), 16(6), 1202-8
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A number of spin-labeled acyl derivs. of atractyloside, (m,n)acyl-ATR (general formula: $CH_3(CH_2)_mCX(CH_2)_nCOO$-ATR, where X is an oxazolidine ring containing a nitroxide), were synthesized and used to probe the ADP carrier in heart mitochondria. They inhibit ADP transport with the same efficiency as unlabeled acyl-ATRs. The inhibition is a mixed competitive and noncompetitive inhibition. The long chain acyl-ATRs ((10,3)-, (7,6)-, (7,8)-, and (5,10)acyl-ATRs) and also the short chain (0,2)acyl-ATR, when added at low concns. to heart mitochondria, give rise to more immobilized ESR spectra than when added to liposomes. On addition of atractyloside or of other specific ligands, spin-labeled long-chain acyl-ATRs bound to the ADP carrier are displaced from their binding site toward the lipid phase of the mitochondrial membrane and the short chain (0.2)acyl-ATR is released into the aqueous phase. Spin-labeled long-chain acyl-ATRs do not show any evidence of binding to a protein when incubated with inside out submitochondrial particles, in spite of the fact that these particles are able to transport ADP. These results are discussed with respect to the size and the asymmetry of the ADP carrier in the mitochondrial membrane and the mechanism of ADP transport.
IT **63193-89-5 63193-90-8 63193-91-9 63193-92-0 63193-93-1 63196-04-3**
RL: BIOL (Biological study)
(as mitochondrial membrane probe)
RN 63193-89-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[7-(4,4-dimethyl-2-octyl-3-oxy-2-oxazolidinyl)-1-oxoheptyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L20 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 K

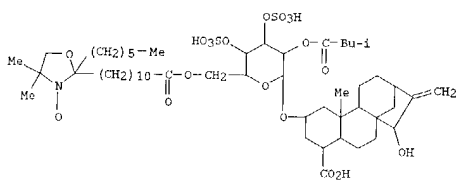
RN 63193-90-8 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-[9-(4,4-dimethyl-2-octyl-3-oxy-2-oxazolidinyl)-1-oxononyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)



●2 K

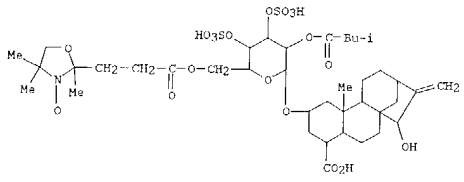
RN 63193-91-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[11-(2-hexyl-4,4-dimethyl-3-oxy-2-oxazolidinyl)-1-oxoundecyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L20 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 K

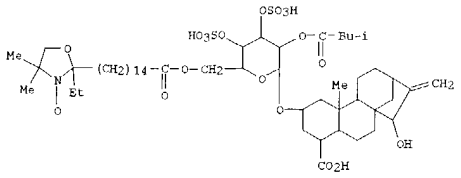
RN 63193-92-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-hydroxy-2-[[2-O-(3-methyl-1-oxobutyl)-6-O-[1-oxo-2-(2,4,4-trimethyl-3-oxy-2-oxazolidinyl)propyl]-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)



●2 K

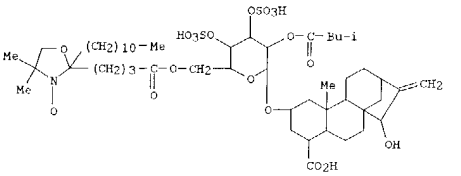
RN 63193-93-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[15-(2-ethyl-4,4-dimethyl-3-oxy-2-oxazolidinyl)-1-oxopentadecyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L20 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



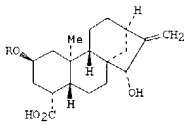
●2 K

RN 63196-04-3 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-(4,4-dimethyl-3-oxy-2-undecyl-2-oxazolidinyl)-1-oxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)



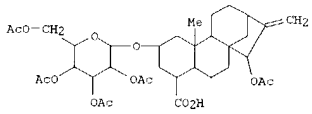
●2 K

L20 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:73060 CAPLUS
DOCUMENT NUMBER: 86:73060
TITLE: The structures of the "coffee atractylosides"
AUTHOR(S): Obermann, Hugo; Spiteller, Gerhard
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Goettingen, Goettingen, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1976), 109(10), 3450-61
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



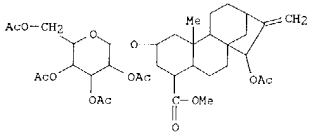
I

AB The atractylosides, isolated from Coffea arabica, have structures I (R = β-D-glucopyranosyl, 3-O-β-D-glucopyranosyl-2-O-isovaleryl-β-D-glucopyranosyl) based on chemical and spectral data.
IT **61773-42-0P 61773-43-1P 61773-48-6P**
**61773-49-7P 61773-50-0P 61773-51-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 61773-42-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-(acetyloxy)-2-[[2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

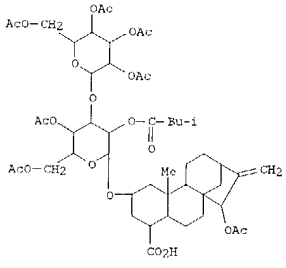


RN 61773-43-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-(acetyloxy)-2-[[2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl]oxy]-, methyl ester, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L20 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

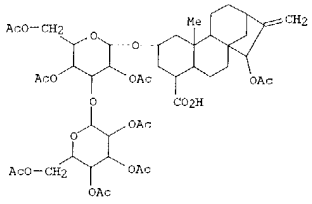


RN 61773-48-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-(acetyloxy)-2-[[4,6-di-O-acetyl-2-O-(3-methyl-1-oxobutyl)-3-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

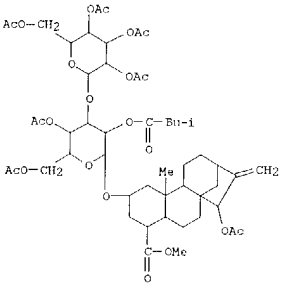


RN 61773-49-7 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-(acetyloxy)-2-[[2,4,6-tri-O-acetyl-3-O-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)-β-D-glucopyranosyl]oxy]-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L20 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

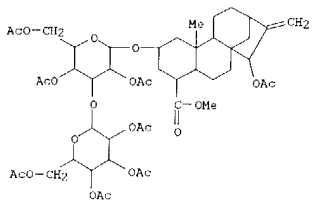


RN 61773-50-0 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-(acetyloxy)-2-[[4,6-di-O-acetyl-2-O-(3-methyl-1-oxobutyl)-3-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)-β-D-glucopyranosyl]oxy]-, methyl ester, (2β,4α,15α)- (9CI) (CA INDEX NAME)



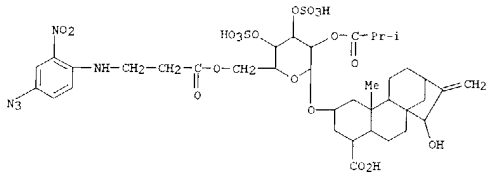
RN 61773-51-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-(acetyloxy)-2-[[2,4,6-tri-O-acetyl-3-O-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)-β-D-glucopyranosyl]oxy]-, methyl ester, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L20 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L20 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN

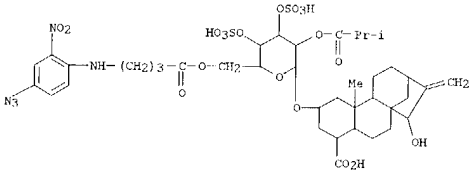
ACCESSION NUMBER: 1976:572971 CAPLUS
DOCUMENT NUMBER: 85:172971
TITLE: Aryl-azido atractylosides as photoaffinity labels for the mitochondrial adenine nucleotide carrier
AUTHOR(S): Lauquin, Guy; Brandolin, Gerard; Vignais, Pierre
CORPORATE SOURCE: Dep. Rech. Fondam./Biochim., CEN, Grenoble, Fr.
SOURCE: FEBS Letters (1976), 67(3), 306-11
CODEN: FEBLAL; ISSN: 0014-5793
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB A photoactive arylazido derivative of atractyloside was used to label covalently the ADP carrier in rat heart mitochondria. The synthesis of 6'[4N(4-azido-2-nitrophenyl)amino]butyrylatractyloside (I) and its propionyl analog is described. I competitively inhibits ADP transport with the same efficiency as atractyloside and competes with atractyloside for binding to mitochondria. The nitrene derivative formed on irradiation of I
binds covalently to mitochondria. By this means, the ADP carrier protein was characterized by Na dodecyl sulfate-polyacrylamide gel electrophoresis; its mol. weight is .apprx.30,000.
IT **60792-98-5 60792-99-6**
RL: BIOL (Biological study)
(ADP carrier protein binding and photolabeling by)
RN 60792-98-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[3-[(4-azido-2-nitrophenyl)amino]-1-oxopropyl]-2-O-(2-methyl-1-oxopropyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)



●2 K

RN 60792-99-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[(4-azido-2-nitrophenyl)amino]-1-oxobutyl]-2-O-(2-methyl-1-oxopropyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, dipotassium salt, (2β,4α,15α)- (9CI) (CA INDEX NAME)

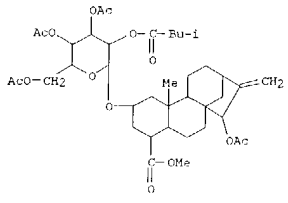
L20 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 K

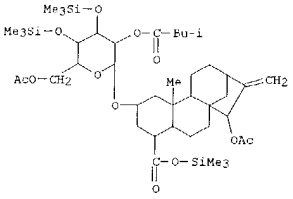
L20 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1974:413746 CAPLUS
DOCUMENT NUMBER: 81:13746
TITLE: Mass spectrometry of atractyloside derivatives. Determination of the number of substituents by a combination of acetylation and silylation
AUTHOR(S): Defaye, G.; Ulrich, J.
CORPORATE SOURCE: D.R.F./Biochim., Cent. Etud. Nucl. Grenoble, Grenoble, Fr.
SOURCE: Organic Mass Spectrometry (1974), 8, 89-94
CODEN: ORMSBG; ISSN: 0030-493X
DOCUMENT TYPE: Journal
LANGUAGE: French
AB The substituents in atractyloside, apoatractyloside, and gummiferin were enumerated from mass spectra of derivatives in which all the functions were silylated or in which the alcs. were acetylated whilst the sulfates and acids were silylated.
IT **42011-33-6 52887-63-5**
RL: PRP (Properties)
(mass spectrum of)
RN 42011-33-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-(acetyloxy)-2-[[3,4,6-tri-O-acetyl-2-O-(3-methyl-1-oxobutyl)-β-D-glucopyranosyl]oxy]-, methyl ester, (2β,4α,15α)- (9CI) (CA INDEX NAME)



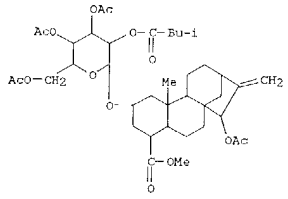
RN 52887-63-5 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-(acetyloxy)-2-[[6-O-acetyl-2-O-(3-methyl-1-oxobutyl)-3,4-bis-O-(trimethylsilyl)-β-D-glucopyranosyl]oxy]-, trimethylsilyl ester, (2β,4α,15α)- (9CI) (CA INDEX NAME)

L20 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



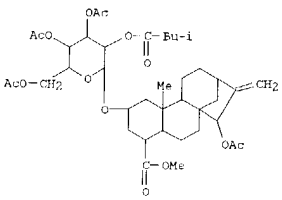
L20 ANSWER 24 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1973:405532 CAPLUS
DOCUMENT NUMBER: 79:5532
TITLE: Stereochemistry of the glycosidic bond of atractyloside
AUTHOR(S): Defaye, Genevieve; Horton, Derek; Wander, Joseph D.
CORPORATE SOURCE: Dep. Rech. Fondam., C.E.N., Grenoble, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1973), (2)(Pt. 2), 615-17
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB The β-D-glucopyranoside structure with C1 conformation was confirmed for atractyloside (I) by PMR of its desulfonated derivative II. II was prepared by desulfonating I with 1% HCl-MeOH, acetylating the OH groups, and esterifying. The desulfonation proceeded with ≤5% anomerization.
IT **42011-33-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(PMR of, glycosidic bond stereochemistry in relation to)
RN 42011-33-6 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-(acetyloxy)-2-[[3,4,6-tri-O-acetyl-2-O-(3-methyl-1-oxobutyl)-β-D-glucopyranosyl]oxy]-, methyl ester, (2β,4α,15α)- (9CI) (CA INDEX NAME)



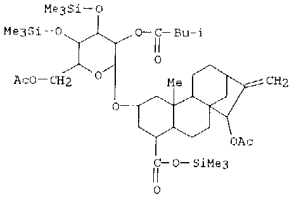
L20 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1972:154082 CAPLUS
DOCUMENT NUMBER: 76:154082
TITLE: Experimental evidence for the identity of gummiferin with carboxyatractyloside
AUTHOR(S): Defaye, Genevieve; Vignais, Paulette M.; Vignais, Pierre V.
CORPORATE SOURCE: Lab. Biochem., C.E.N. Grenoble, Grenoble, Fr.
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences, Serie D: Sciences Naturelles (1971), 273(25), 2671-3
CODEN: CHDDAT; ISSN: 0567-655X
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB The mass spectra of acetylated and trimethylsilylated derivs. of gummiferin (I) and carboxyatractyloside (II) were essentially identical. A comparison of the NMR spectra of the Me esters of I and II indicated that I contained 2 CO2H groups while II contained only 1. Pyrolysis of I gave II. These results were compared with the electrophoretic and chromatog. properties of I and II and their structures were assigned.
IT **35959-30-9 35988-25-1**
RL: PRP (Properties)
(mass spectrum of)
RN 35959-30-9 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 15-(acetyloxy)-2-[[3,4,6-tri-O-acetyl-2-O-(3-methyl-1-oxobutyl)-α-D-glucopyranosyl]oxy]-, methyl ester, (2β,4α,15α)- (9CI) (CA INDEX NAME)

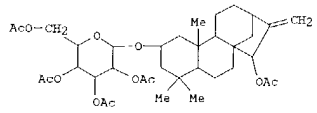


RN 35988-25-1 CAPLUS
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-acetyl-2-O-(3-methyl-1-oxobutyl)-3,4-bis-O-(trimethylsilyl)-α-D-glucopyranosyl]oxy]-15-(acetyloxy)-, trimethylsilyl ester, (2β,4α,15α)- (9CI) (CA INDEX NAME)

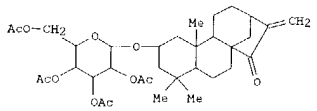
L20 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L20 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1971:515874 CAPLUS
DOCUMENT NUMBER: 75:115874
TITLE: Structures of creticosides A and B, two new diterpenoid glucosides from Pteriscretica
AUTHOR(S): Chen, Chiu-Ming; Murakami, Takao
CORPORATE SOURCE: Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1971), 19(7), 1495-8
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Examination of the rhizome of P. cretica yielded 2 new diterpenoid glucosides; these new glucosides were named creticoside A(I) and creticoside B (II). The structures and phys. characteristics are reported.
IT **34539-69-0P 34539-71-4P 34539-72-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 34539-69-0 CAPLUS
CN Creticoside A, pentaacetate (8CI) (CA INDEX NAME)

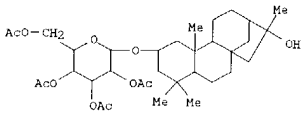


RN 34539-71-4 CAPLUS
CN Kaur-16-en-15-one, 2β-(β-D-glucopyranosyloxy)-, tetraacetate (8CI) (CA INDEX NAME)



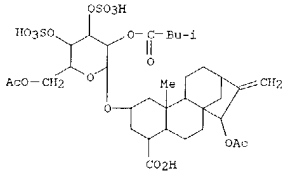
RN 34539-72-5 CAPLUS
CN Creticoside B, 2,3,4,6-tetraacetate (8CI) (CA INDEX NAME)

L20 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



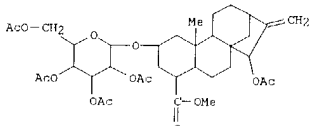
L20 ANSWER 27 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1967:517201 CAPLUS
DOCUMENT NUMBER: 67:117201
TITLE: Structure of atractyloside
AUTHOR(S): Piozzi, Franco; Quilico, Adolfo; Fuganti, Claudio; Ajello, Tommaso; Sprio, Vincenzo
CORPORATE SOURCE: Univ. Palermo, Palermo, Italy
SOURCE: Gazzetta Chimica Italiana (1967), 97(6), 935-54
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: Italian
GI For diagram(s), see printed CA Issue.
AB A structure is assigned to the title compound (I), m. 157-8° (decomposition) [α]D -53° (c 1.1, H2O), is obtained from Atractylis gummifera roots according to known procedures. I (3.07 g.) in a mixture of 100 ml. water and 200 ml. EtOH is hydrogenated in the presence of 200 ml. 10% Pd/C to give dihydroatractyloside, m. 172-3°, [α]D -34.5° (c 1.0, H2O). A mixture of 300 ml. M H3PO4 and 1.606 g. I is heated to give isovaleric acid. A solution of 200 mg. I in M H2SO4 is refluxed 4 hrs. to give D-glucose (II). A solution of 1.6 g. I in 20 ml. 20% KOH is refluxed 8 hrs., diluted with 80 ml. water, cooled, and acidified with 10% HCl to give atractyligenin (III), m. 180°. Similarly prepared is hydroatractyligenin, m. 236-7° (EtOAc). A solution of 1 g. I in 5 ml. pyridine and 5 ml. Ac2O is kept 24 hrs. to give di-O-acetylatractyloside (IV). A solution of 2 g. I in 40 ml. water containing 2 g. Ba(OH)2 is heated to give apo-atractyloside (V) Ba salt, m. 155° (decomposition), which is converted to V di-K salt, m. 232-4°. A mixture of 3 g. V Ba salt, 100 g. 1% Na amalgam, 20 ml. water, and 80 ml. MeOH is agitated 72 hrs. and the product is treated with CH2N2 to give penta-O-acetylatractyline Me ester (VI), m. 165-7° (EtOH). A mixture of 2 g. of I, 2 ml. concentrated HCl, and 200 ml. MeOH is kept 24 hrs. and the product is treated with CH2N2 to give isovalerylatractyline Me ester (VII), m. 112-14°. A mixture of 200 ml. VII, 20 ml. 5% Ba(OH)2, and 20 ml. MeOH is heated 10 min. at 70-80°, CO2 is introduced into the mixture, and the product is treated with CH2N2 to give atractyline Me ester (VIII), m. 130-2°; VII is treated with Ac2O and pyridine to give VI m. 165-7° (EtOH). A mixture of 800 ml. IV, 0.8 ml. concentrated HCl, and 80 ml. MeOH is kept 24 hrs. and the product is treated with CH2N2 to give di-O-acetylisovalerylatractyline Me ester (IX), m. 108°. A mixture of 100 ml. VIII and 5 ml. 20% KOH is refluxed 6 hrs. to give III; a mixture 100 ml. VIII and 5 ml. M H2SO4 is refluxed 4 hrs. to give II. I, V di-K salt, V Ba salt, VII, atractyline Me ester, and VI give neg. Fehling tests. A solution of 1 g. hydroatractyloside in EtOH is treated with CH2N2, the EtOH is removed, the product is dissolved in 20 ml. HOAc, a solution prepared from 200 ml. CrO3, 5 ml. HOAc, and 0.1 ml. water is added in about 10 min., and the mixture is refluxed with 100 ml. 20% KOH to give about 20% 15-oxohydroatractyligenin Me ester, m. 124°; monoacetyl derivative m. 159°. Results for the HIO4 titration of I, V di-K salt, atractyline Me ester, VII, X, Me α-D-glucopyranoside and Me 4,6-O-benzylidene-α-D-glucopyranoside are given. A solution of 5 g. I and 25 ml. HCONMe2 is treated with 5 g. Ag2O and 10 ml. MeI, the mixture is agitated 24 hrs. and added to 200 ml. MeOH, the mixture is evaporated to dryness, and 200 ml. 2N H2SO4 is added. The mixture is refluxed 12 hrs., BaCO3 is added at 40-50°, and the product is treated with 5 ml. Ac2O and 5 ml. pyridine to give about 600 ml. product. Gas phase chromatog. shows that the product contains 1,2,3,4,6-penta-O-acetyl-D-glucose, 3-O-methyl-1,2,4,6-tetra-O-acetyl-D-glucose, 2-O-methyl-1,3,4,6-tetra-O-acetyl-D-glucose (X), 4-O-methyl-1,2,3,6-tetra-O-acetyl-D-glucose,

L20 ANSWER 27 OF 27 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
6-O-methyl-1,2,3,4-tetra-O-acetyl-D-glucose (XI), 2,3-di-O-methyl-1,4,6-tri-O-acetyl-D-glucose, and 2,3,4,6-tetra-O-methyl-1-O-acetyl-D-glucose (XII). V gives a mixt. contg. XII, XI, X, and a di-O-methyl-tri-O-acetyl-D-glucose. Atractyline Me ester gives XII.
IT **18466-99-4P 18467-00-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 18466-99-4 CAPLUS
CN Atractyloside, diacetate, dipotassium salt (8CI) (CA INDEX NAME)



●2 K

RN 18467-00-0 CAPLUS
CN Atractylin, methyl ester, pentaacetate (8CI) (CA INDEX NAME)



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| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 129.30 | 694.24 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | -18.71 | -47.82 |

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